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# **NASA.....MSU**

**STATUS REPORT  
MARCH 1, 1995 - NOVEMBER 30, 1995**

**NASA GRANT NAG 5-2375**

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## INTRODUCTION

This document represents a progress report of our research on the grant (NAG 5-2375) from NASA between March 1, 1995 and November 30, 1995. During this reporting period our laboratory concentrations consisted of several parts; (1) We made several presentations of the work sponsored by NASA covered under the last status report period. (2) We irradiated and successfully completed Moessbauer measurements on a high temperature superconductor. (3) We continued the improvement of our laboratory with the development of improved software and (4) we made modifications of equipment to increase the efficiency and decrease the time necessary for completing an experimental investigation. In addition to our research results, this report contains a copy of the last financial report submitted by the University's business office that was related to this grant. It shows the expenditures as of September 30, 1995. We plan to expend all of the funds by the end of the grant period.

## **RESULTS OF INVESTIGATIONS**

### **Irradiation Studies**

High temperature superconductors have made large scale technical applications a possible reality. However, they have some limitations. Among them are their limited critical currents and low current density. Previous experimental work indicated that irradiation by neutrons were effective in increasing the measured current density while reducing current density anisotropy and transition temperatures. Continued research in this area may ultimately yield a high temperature superconductor with a high enough current density that it becomes practical in technical applications. We wanted to see if we could use Moessbauer spectroscopy to see if we could observe any changes in the irradiated superconductors and to interpret the causes of the observations. We chose to look at the Moessbauer parameters linewidth and isomer shift. The linewidth gives one an indication of the number of different sites in the material and the isomer shift is related to the electronic charge density at the nucleus.

To carry out the above objective one-half of a superconductor sample ( $\text{EuBa}_2\text{Cu}_3\text{O}_{7-x}$ ) was irradiated by a one curie plutonium beryllium neutron source with approximately  $3.45 \times 10^{13}$  neutrons. The other half was used as the control and thus was not altered in any way. Moessbauer spectra were taken for both halves. The calculated isomer shift and linewidths for the irradiated and the

non-irradiated sample are listed in Table 1. Europium fluoride was used as a standard for the isomer shift calculations and iron foil was used to calibrate the system. Figures 1 and 2 show the Moessbauer spectra of the non-irradiated and irradiated samples respectively.

TABLE 1

<u>Sample</u>	<u>Linewidth Ratio</u>	<u>Isomer shift (mm/s)</u>
EuF <sub>3</sub>	1	0
EuBa <sub>2</sub> Cu <sub>3</sub> O <sub>7-x</sub>	.90 + .05	-.82 + .01
EuBa <sub>2</sub> Cu <sub>3</sub> O <sub>7-x</sub> (irradiated)	.85 + .05	-.94 + .01

The difference between the linewidth ratio of the irradiated and non-irradiated samples of EuBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> does not deviate beyond the experimental error. This indicates that all the europium atomic sites are similar. In the case of the isomer shift however, we see a difference that infers that neutron irradiation substantially alters its isomer shift. This implies that there is an increase in the s electron density at the nucleus of the europium atom. This results suggests to get a higher current density in superconducting materials, one needs to modify the superconductor to increase its s electron density. We have requested a larger dosage of neutrons from the nuclear reactor at NIST and we are waiting for a reply to our request. We want to see what happens for a larger dosage of neutrons.

#### Phonon Studies

We reported on our previously observed phonon anomaly (1) in a Bi high T<sub>c</sub> compound at the March 1995 American Physical Society meeting in Washington D.C. (2). This work indicated that other sites besides the commonly accepted copper planes are effected by the superconductivity mechanism.

#### Particle Size Studies

In an attempt to gain a better understanding of the cause of superconductivity, we were part of a group effort looking at the relationship of starting particle size with the final superconductor. We wanted to see if there was any relationship between starting particle size and the Moessbauer parameters of linewidth and isomer shift. Measurements were made on a number of EuBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> superconductors prepared by a solid state reaction of Eu<sub>2</sub>O<sub>3</sub>, BaCO<sub>3</sub>, and CuO powders. The letter designation for each particle size was used to name the pellets, with the first letter corresponding to Eu<sub>2</sub>O<sub>3</sub>, the second to BaCO<sub>3</sub>, and the third to CuO.

For example, the sample BAB is 100 - 200 mesh size  $\text{Eu}_2\text{O}_3$ , above 100 mesh size  $\text{BaCO}_3$ , and 100 - 200 mesh size  $\text{CuO}$ . The particle size relates to the diameter of the particles of that mesh. Table 2 shows the relationship of particle size and letter designation.

**TABLE 2** - Mesh Sizes and Nomenclature

<u>Mesh Size</u>	<u>Letter Designation</u>	<u>Particle Size</u>
above 100	A	>150 $\mu\text{m}$
100 - 200	B	75 $\mu\text{m}$ - 150 $\mu\text{m}$
200 - 325	C	45 $\mu\text{m}$ - 75 $\mu\text{m}$
325 - 400	D	38 $\mu\text{m}$ - 45 $\mu\text{m}$

Spectra were taken in transmission geometry at room temperature in the constant acceleration mode and were fitted by a least squares lorentzian analysis program. Table 3 shows the linewidth and isomer shift for the various superconductors. Europium fluoride was used as a standard for isomer shift calculations. Figure 3 shows the experimental spectrum for  $\text{EuF}_3$ . An iron foil was used to calibrate the system and its spectrum is shown in Figure 4. Figures 5 through 10 show the Moessbauer experimental data for the various particle sizes.

The experimental results do not show a relationship between linewidth and particle size. All of the isomer shifts give the same results within experimental error. This is understandable since particle size is a macroscopic specification whereas linewidth and isomer shift are microscopic applications. Different starting particle size does not effect the final product when investigated with Moessbauer spectroscopy. This is similar to the conclusion of Howard in his study on the relationship between particle size and transition temperature for high  $T_c$  compounds(3). A paper including this work is being prepared for submission for publication (4).

## SOFTWARE DEVELOPMENT

During this reporting period, we developed several new computer subroutines to reduce the tedious task of analyzing data. We developed a code that generated a least squares fit of the parabola that appeared in the Moessbauer spectrum due to the changing solid angle the detector sees because of the motion of the source, our program strips the parabola off the spectrum. This procedure will accelerate the convergence of the lorentzian fitting code. Figure 5 is a plot showing the original data along with flat data after subtracting the parabola. A copy of this code is found in Appendix B. We also developed a code using the graphing software called MAT LAB to do the fitting of Moessbauer data. The advantage of MAT LAB is that we can now use a pc instead of the University's mainframe computer to analyze our experimental data. We found this program to give us the same results as that found using the mainframe. This capability will free our research laboratory from the restrictions imposed by using the University's

computing system. We plan to submit this program for publication in a computer physics journal. A copy of this code is found in Appendix B. The third major program represents an improvement of our computer program for plotting the final plots of experimental Moessbauer data. We modified the software provided by the company who designed our Moessbauer system (Austin Science) into one that plots absorption versus velocity and gives us camera ready spectra for publication. A comparison of the two different computer codes may be observed by comparing the horizontal axis of figures 3 and 4 (Austin Science) with Figures 1,2,5,6,7,8,9,10.

#### REFERENCES

1. Oliver, F.W., NASA Annual Report, Oct. 1, 1993-Sept. 30, 1994, Grant# NAG 5-2375.
2. Oliver, F.W., Hoffman, E., Tarleton, D., May, L., Violet, C.E., and Seehra, M.S., April A.P.S. meeting, Washington, D.C.
3. Edwards, M.A., Howard, J.W., private communication.
4. Edwards, M.A., Howard, J. W., Radcliffe, D., Wynter, C.I., Oliver, F.W., et al., (To be submitted to Physica C).

M.S.U. PHYSICS 12-01-1995 Time: 00:29:49

a: \b575mp30.dat, calibrated using a: b577mp.dat and a: \b573mp2.dat  
Superconductor ABB

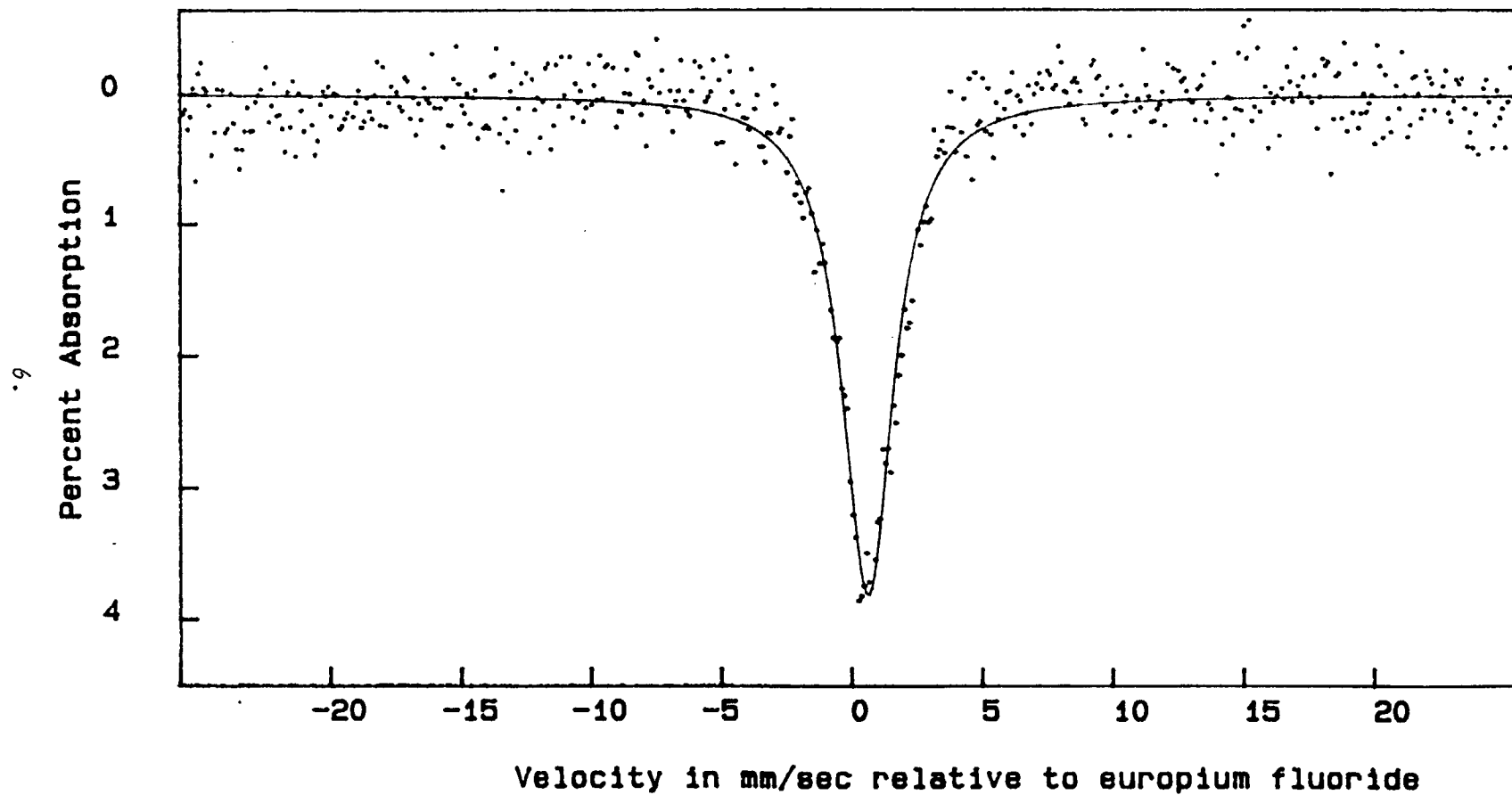


Figure 1

M.S.U. PHYSICS 12-01-1995 Time: 00:48:03

a: \b576mp2.dat, calibrated using a: b577mp.dat and a: \b573mp2.dat  
Superconductor ABB (irradiated)

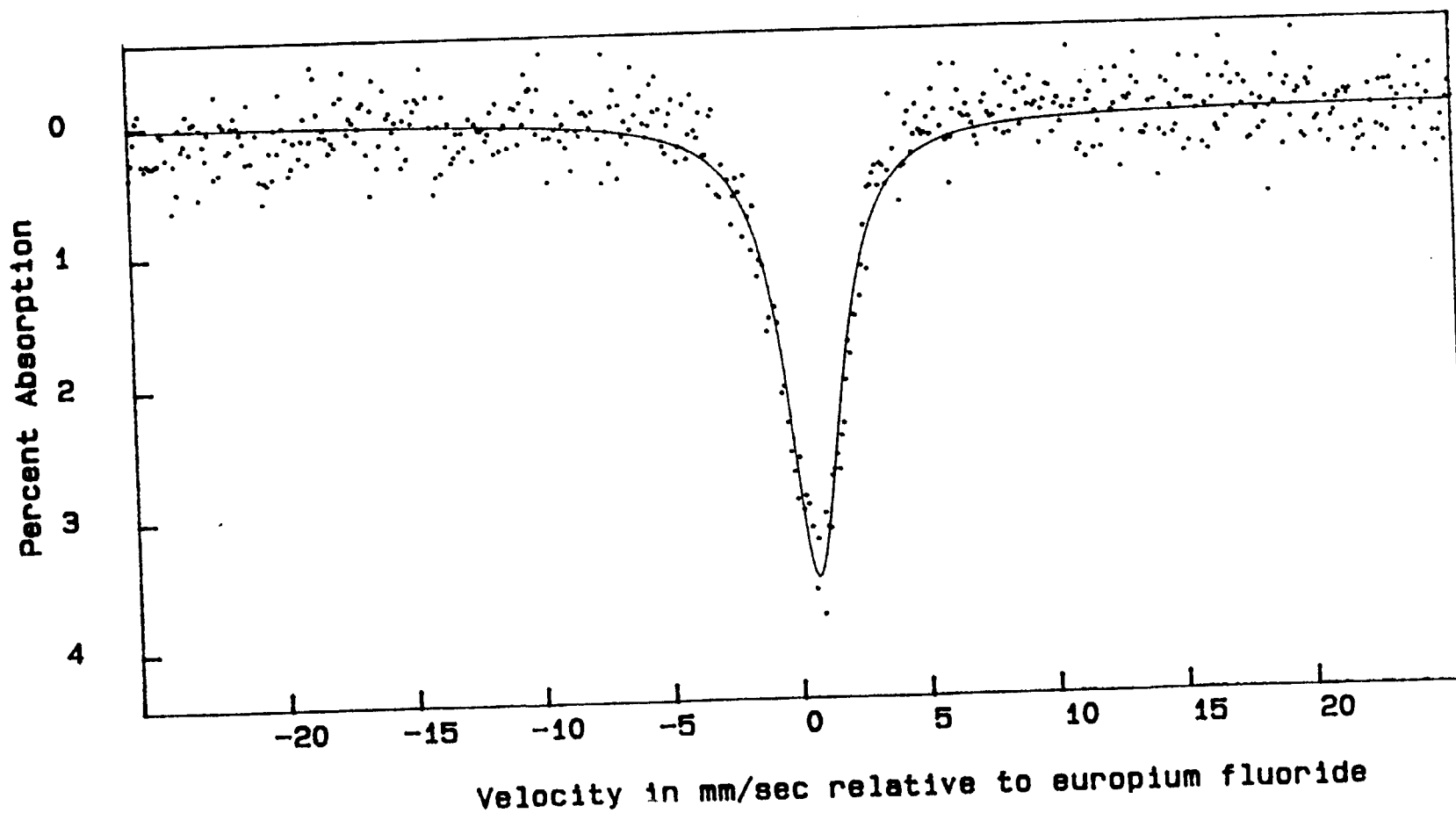


Figure 2



M.S.U. PHYSICS 08-17-1995 Time: 11: 25: 02

A: \B549MP.DAT  
EuF3

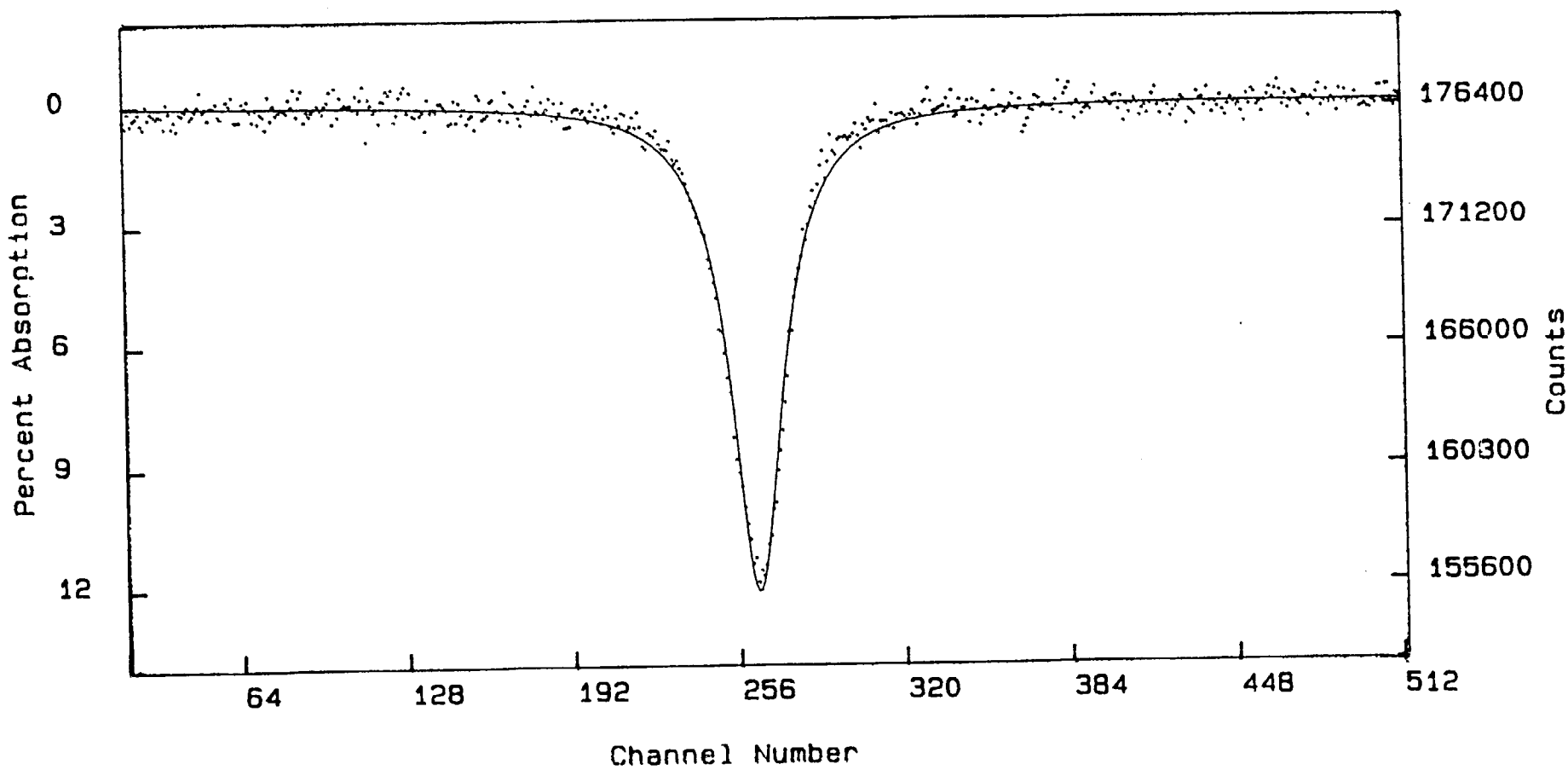


Figure 3

M.S.U. PHYSICS 08-17-1995 Time: 11:33:36

a: \b551mp.dat  
FeFoil

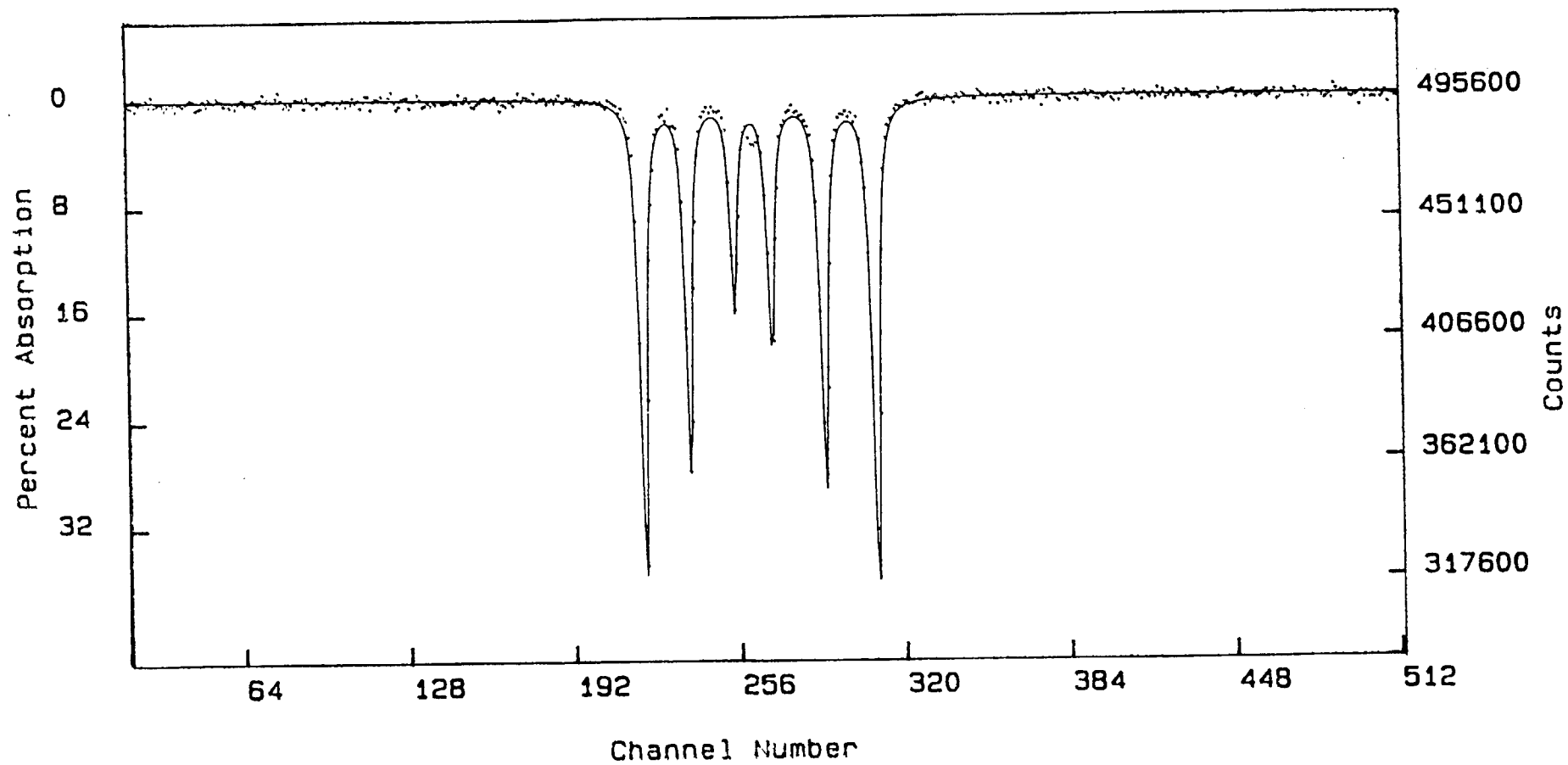


Figure 4

M.S.U. PHYSICS 08-15-1995 Time: 16:45:12

a: \b550mp.dat, calibrated using a: \b549mp.dat and a: \b551.dat  
Superconductor BBA

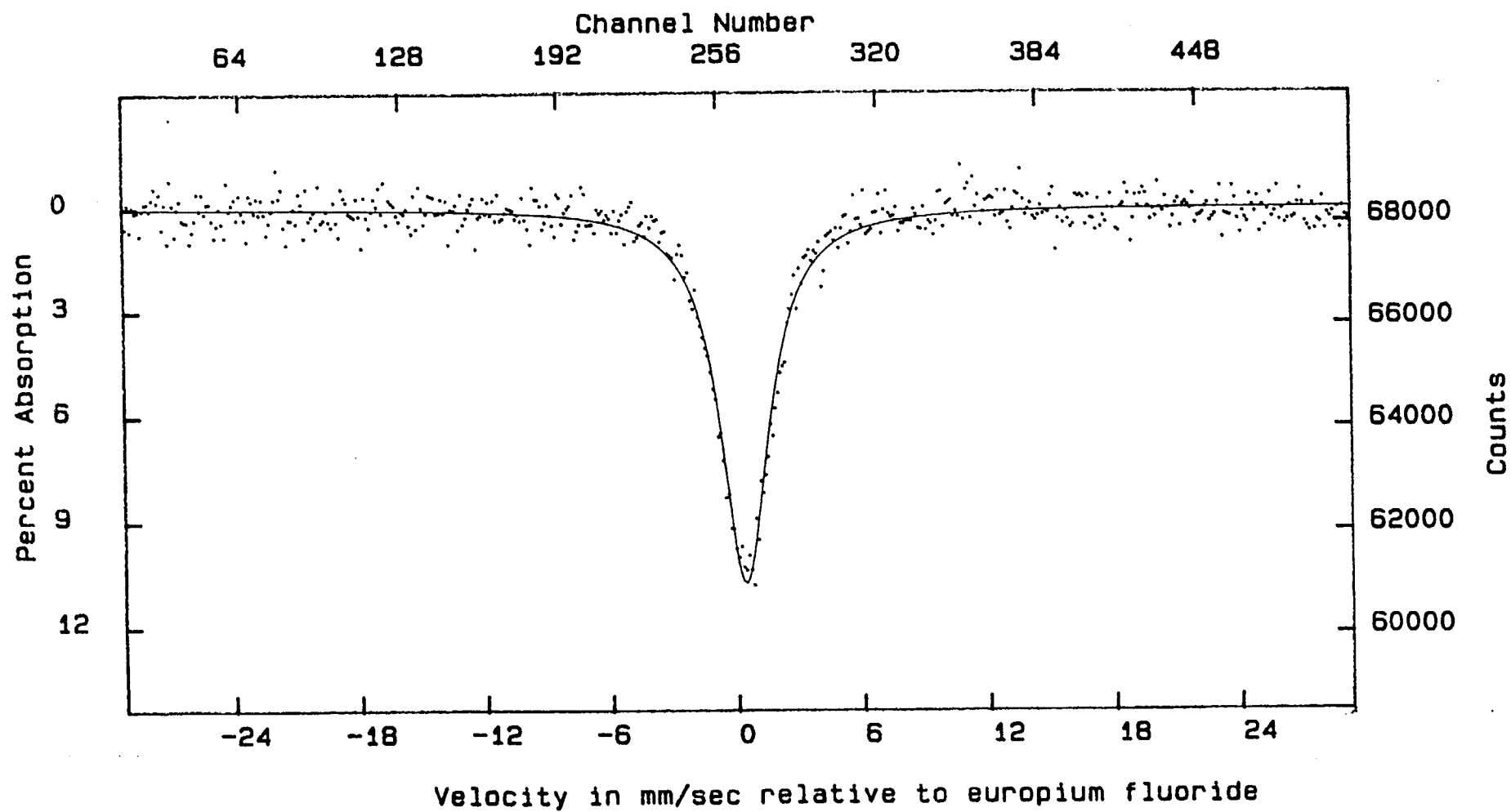


Figure 5

BBA

M.S.U. PHYSICS 08-16-1995 Time: 10:24:42  
 a:\b555mp.dat, calibrated using a:\b549mp.dat and a:\b551.dat  
 Superconductor BBC

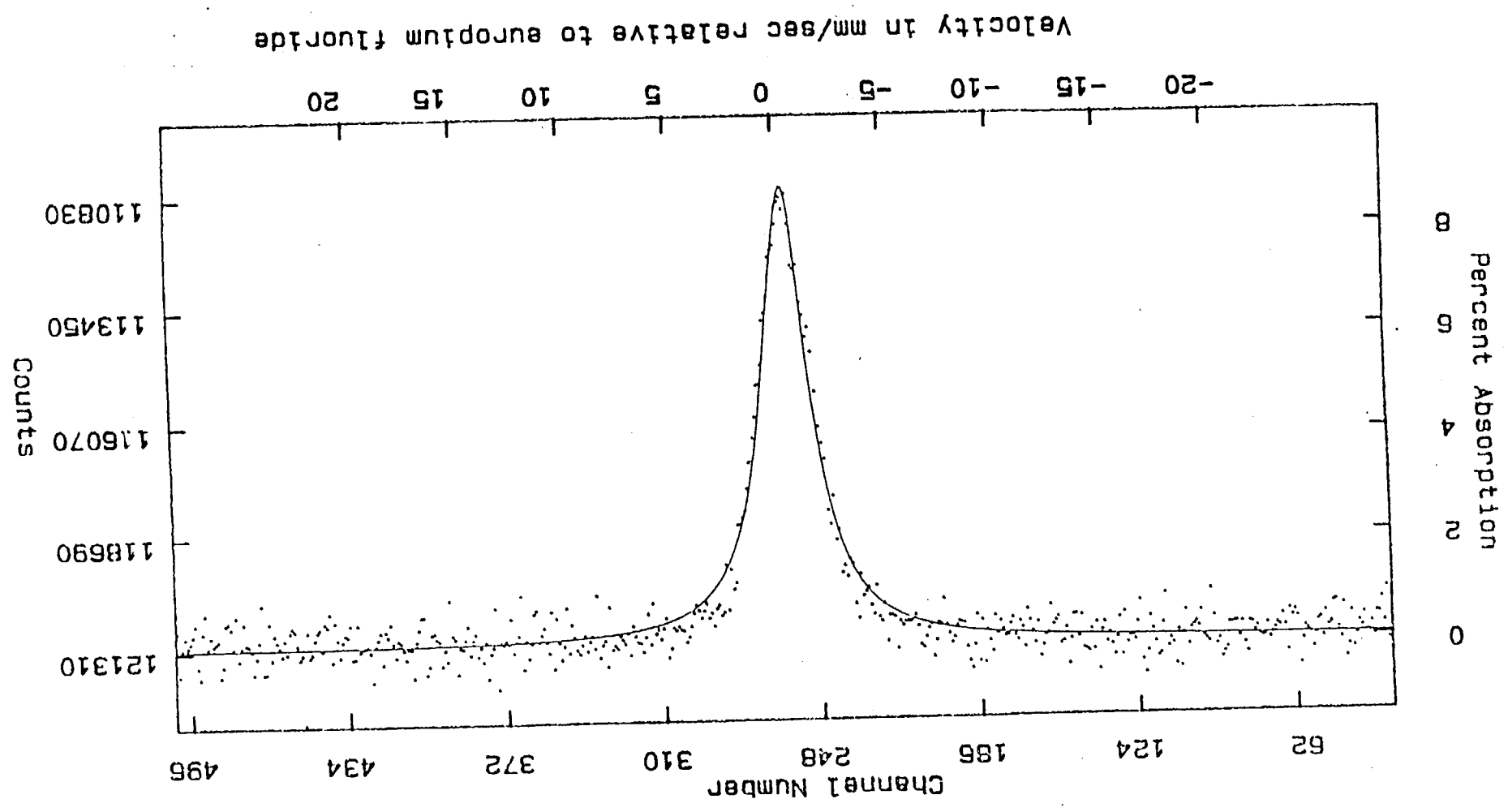


Figure 6

M.S.U. PHYSICS 08-16-1995 Time: 10:31:40

A: \B553MP.DAT, calibrated using a: \b549mp.dat and a: \b551.dat  
Superconductor BBB

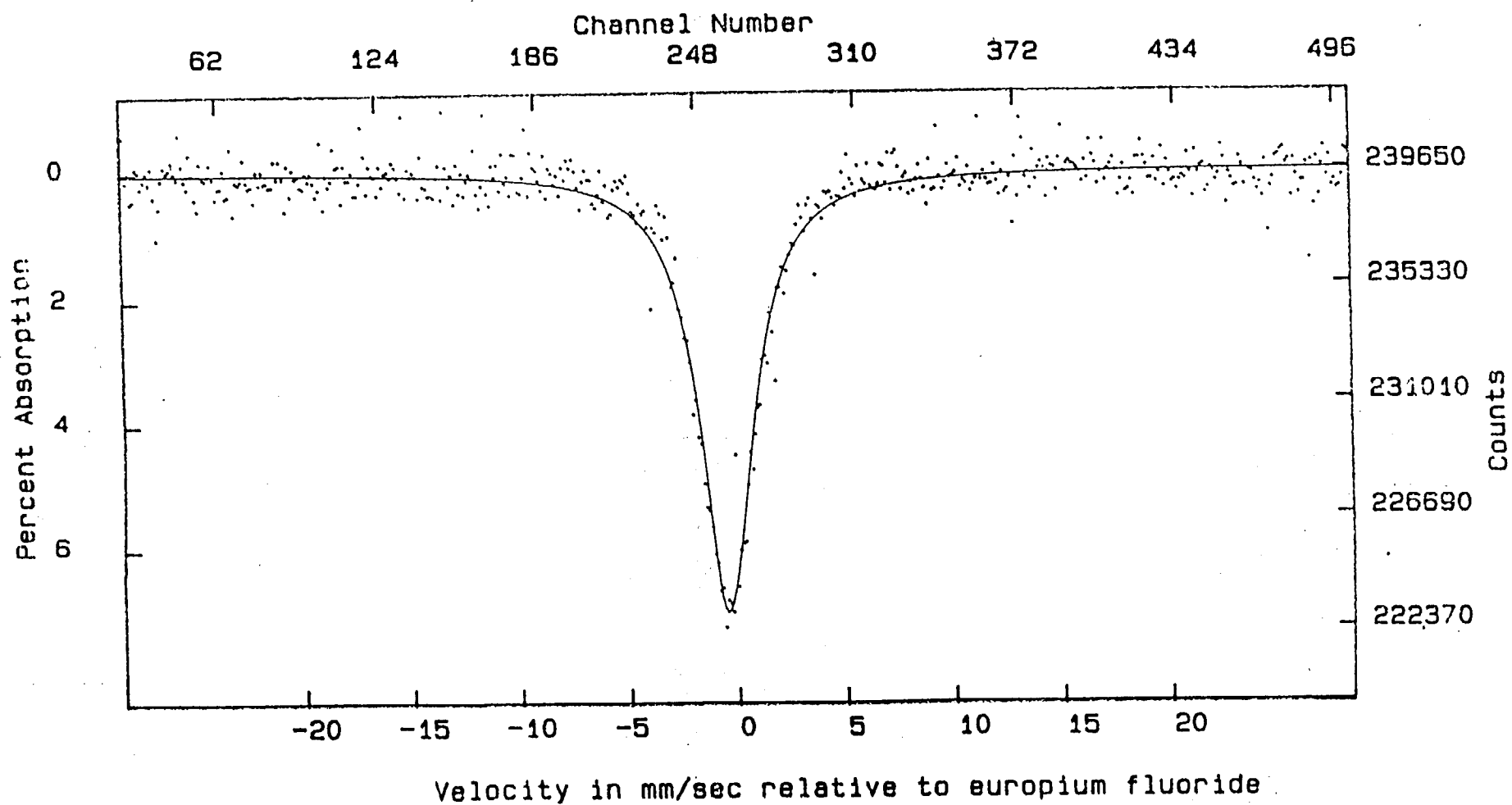


Figure 7

M.S.U. PHYSICS 08-16-1995 Time: 10:38:04

A: \B552MP.DAT, calibrated using a: \b549mp.dat and a: \b551.dat  
Superconductor BAB

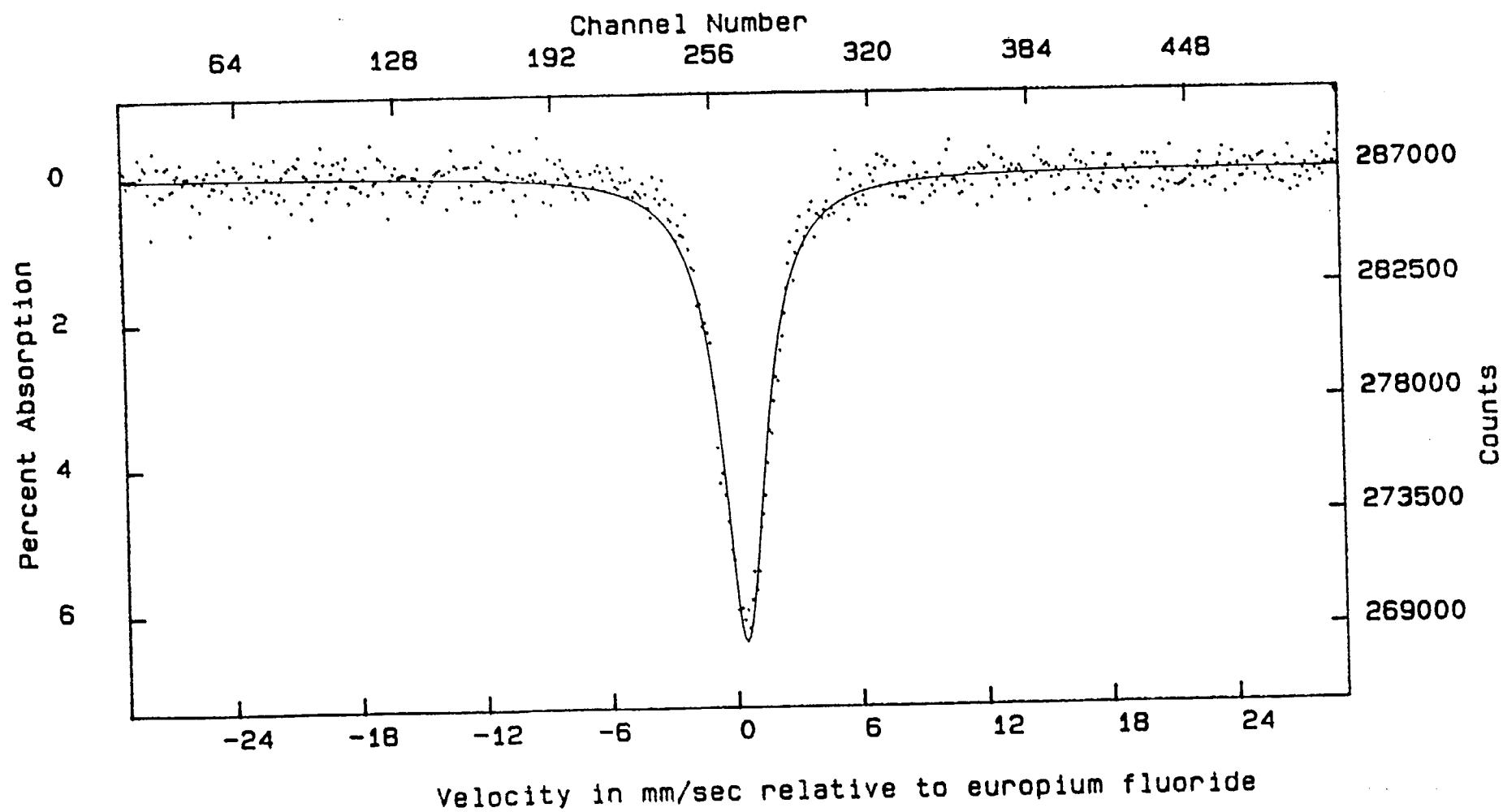


Figure 8

M.S.U. PHYSICS 08-18-1995 Time: 14:46:42

a: \b554mp.dat, calibrated using a: \b549mp.dat and a: \b551.dat  
Superconductor CCD

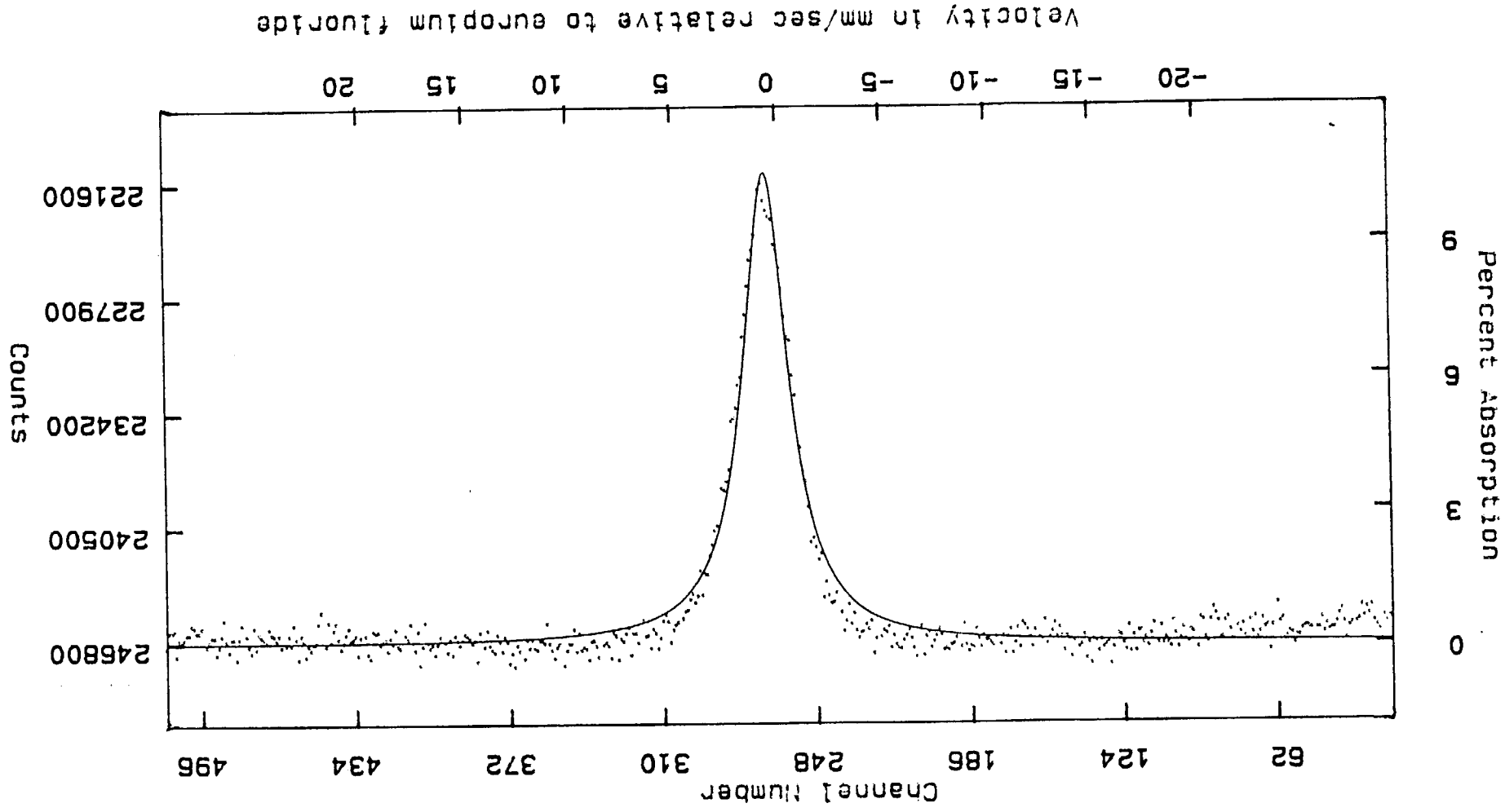


Figure 9

M.S.U. PHYSICS 08-17-1995 Time: 11:13:45

A:\B556MP.DAT, calibrated using A:\B549MP.DAT and A:\B551.DAT  
Superconductor ABB

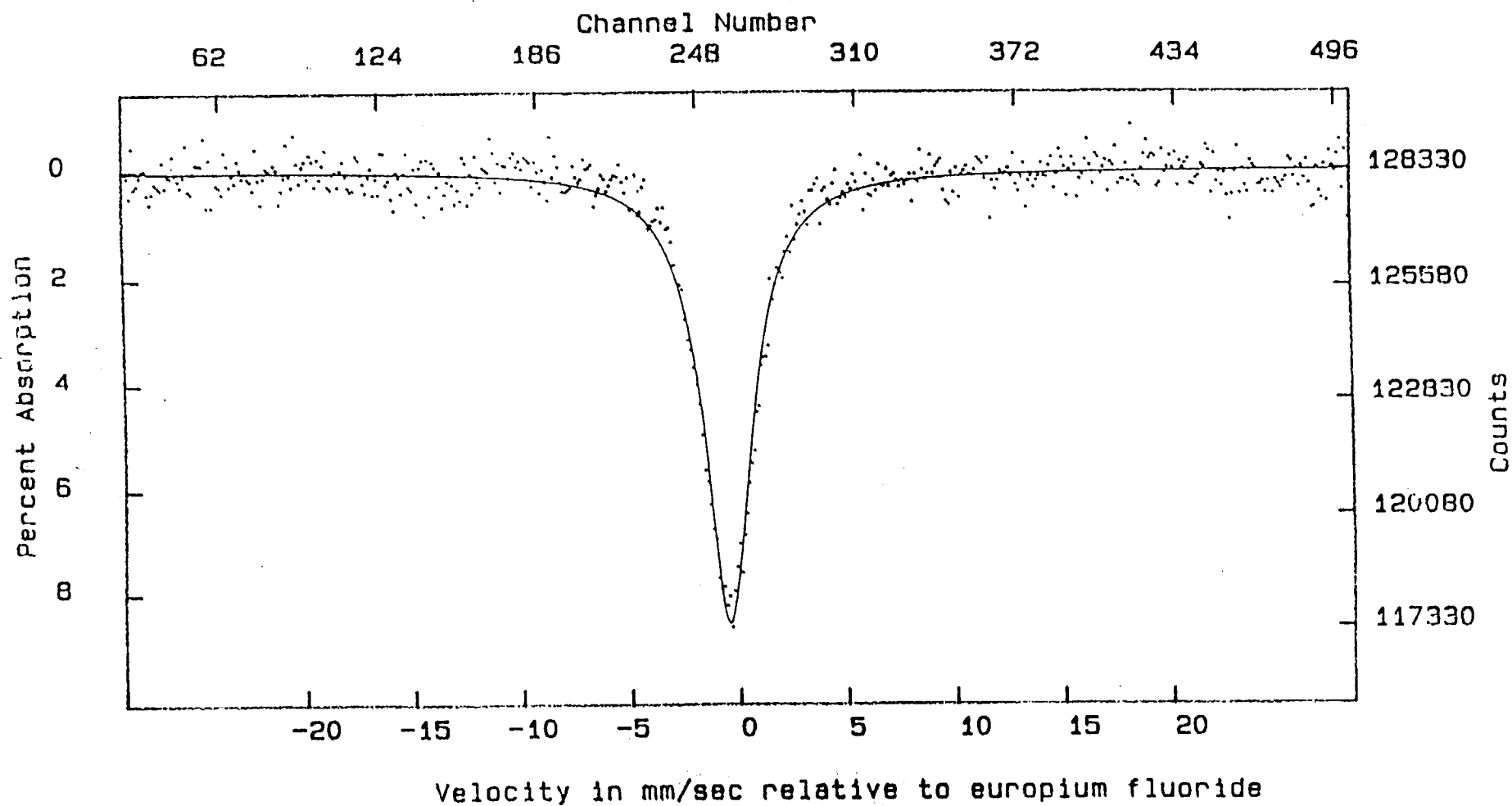


Figure 10



TABLE 3

Sample	L.W (mm/s)	L.W Ratio	I.S
EuF <sub>3</sub>	2.90 ± .05	1	0
BBC	2.67 ± .05	.92	.87 ± .02
BBA	2.83 ± .05	.98	.78 ± .02
BBB	2.92 ± .05	.99	.82 ± .02
BAB	2.58 ± .05	.89	.79 ± .02
CCD	2.66 ± .05	.92	.82 ± .02
ABB	2.61 ± .05	.90	.82 ± .02

L.W ( Line Width)

I.S ( Isomer Shift)

## APPENDIX A - PAPERS PRESENTED

## THURSDAY MORNING

10:00

I10 11

**Determination of Gap Distortion and Longitudinal Resonance Frequency in Superfluid  $^3\text{He-B}$ .** M.R. RAND, D.T. SPRAGUE, T.M. HAARD, J.B. KYCIA, P.J. HAMOT, Y. LEE, D.M. MARKS, W.P. HALPERIN, *Northwestern University* — We have performed pulsed transverse nuclear magnetic resonance in superfluid  $^3\text{He-B}$ . We derived and then numerically solved the Leggett equations for the high field limit. From our experiments and our analysis of the Leggett equations we have determined the temperature dependence of the longitudinal resonance frequency and the distortion of the energy gap. Numerical solutions show that the tipping angle dependent precession frequency generally differs substantially from the prediction of stationary solutions and depends on the magnitude of the transverse tipping field. However, for tipping angles of  $\phi < 60^\circ$  and also for  $\phi \approx 125^\circ$ , the precession frequency agrees with the stationary solution, being insensitive to the magnitude of the tipping field. This work is supported by the National Science Foundation through grants DMR-9314025 and DMR-9311918.

10:12

**Theory of Pulsed NMR Studies in Solid  $\text{D}_2$**  T. DINESEN, B. C. SANCTUARY, *Mc. Gill U.* and H. MEYER, *Duke U.* Density matrix theory is used to calculate the response signal of  $\text{o-D}_2$  (with rotational angular momentum  $J=0$  and nuclear spin  $I=2$ ) in two- and three-pulse NMR experiments. A closed-form method has been successfully applied<sup>1)</sup> to the solid echo properties of  $\text{o-H}_2$  and  $\text{p-D}_2$  (both with  $J=1$  and  $I=1$ ), but had not previously been developed for the  $I=2$  spin system. We find, as expected, similar functional dependence upon the experimental parameters of both ortho and para systems and arrive at a detailed account of the intermolecular dipolar field. While this closed-form method considers individual contributions to the echo amplitude, greater physical insight is gained by considering the rotational invariance properties of the line shape. Results from a spherical tensor and product operator basis are then compared with one another as representations of the quadrupolar solid echo response problem. Finally the predicted solid echo amplitude ratio of the  $I=1$  and  $I=2$  components, expressed as a function of the time  $\tau$  between the pulses and their respective phases  $\Phi$ , is compared with that observed<sup>1)</sup> for several  $\text{D}_2$  crystals of various  $J=1$  concentrations. We also discuss the satellite echoes, predicted for the  $I=2$  system, which have been observed<sup>2)</sup> in  $\text{D}_2$  adsorbed on  $\text{MgO}$  but not<sup>1)</sup> in solid  $\text{D}_2$ .

1) I. Yu *et al.*, *J. Low Temp. Physics* **51**, 369 (1983) for  $\text{H}_2$ .  
D. Clarkson, X. Qin and H. Meyer, *J. Low Temp. Physics* **91**, 119 (1993) for  $\text{D}_2$ .

2) M.P. Volz *et al.* *Phys. Rev. Lett.* **63**, 2582 (1989)

### SESSION I11: DAMOP: ATOMIC AND MOLECULAR STRUCTURE AND SPECTROSCOPY

Thursday morning, 20 April 1995

Room 3 at 8:00

R. Pratt, presiding

8:00

**I11 1 Rovibronic Spectroscopy of the Ethoxy Radical in a Supersonic Jet Environment** PRABHAKAR MISRA, *Howard University* — The ethoxy ( $\text{C}_2\text{H}_5\text{O}$ ) radical is generated as a chemical intermediate in combustion and atmospheric processes. It belongs to the  $\text{C}_s$  point group and has 18 fundamental vibrational frequencies.  $\text{C}_2\text{H}_5\text{O}$  was produced in situ by photolyzing freshly synthesized  $\text{C}_2\text{H}_5\text{ONO}$  in a pulsed supersonic expansion with  $\text{KrF}$  ( $\lambda$  248 nm) excimer laser pulses. A frequency-doubled Nd:YAG-pumped dye laser with a nominal linewidth of  $0.07\text{ cm}^{-1}$  served as the probe beam for excitation of the radical. Extensive laser excitation spectra of jet-cooled  $\text{C}_2\text{H}_5\text{O}$  have been recorded in the 310-350 nm region with  $0.15\text{ cm}^{-1}$  resolution. Wavelength-resolved emission spectra have also been obtained with an Optical Multichannel Analyzer system, which employed CCD detection

in conjunction with a 0.275 m monochromator equipped with a 1200 grooves/mm grating that provided a resolution of 0.5 nm. Several new vibrational frequencies have been identified for the  $\text{C}_2\text{H}_5\text{O}$  radical.

\*Supported by EPA grant R81-9720-010, NASA grant NAG3-1677 and CSTE (NAGW-2950).

8:12

**I11 2  $^{151}\text{Eu}$  Mössbauer Investigation on a Bismuth High- $T_c$  Superconductor.** F. W. Oliver, E. Hoffman, D. Tarleton, *Morgan State Univ.*, L. May, *The Catholic Uni. of America*, C.E. Violet, *L.N.L.*, and M. S. Seehra, *West Virginia Univ.* We report on Mössbauer studies on Bismuth high-temperature superconductors with a particular emphasis on our findings on the superconductor

$\text{Bi}_2\text{Ca}_0.5\text{Eu}_{0.5}\text{Sr}_2\text{Cu}_2\text{O}_x$  using  $^{151}\text{Eu}$ . Magnetic susceptibility measurements show a transition temperature of 87 K. Mössbauer measurements were performed between liquid nitrogen and room temperature. Isomer shift measurements show the Eu to be trivalent and is similar to those found for Eu based 1,2,3 high- $T_c$  superconductors. Evidence of phonon softening is observed about the Eu atom during transition to the superconducting state. A discussion on the isomer shift and f factor as a function of temperature will be reported and compared with previous results found in Eu based high- $T_c$  superconductors.

Supported by NASA - NAG 5-2375.

8:24

I11 3

**Microwave Dielectric Behavior of Transition Metal Oxides.** J. N. DAHIYA, *Southeast Missouri State University*. --A microwave resonant cavity in the  $\text{TE}_{011}$  mode is used to study the dielectric properties of a sample of cobalt oxide and nickel oxide. The microwave data of these crystals is taken as a function of frequency and temperature. A fixed length of the sample is inserted into the resonant cavity and the perturbation of the signal are recorded in terms of the frequency shifts and width changes. Slater's perturbation equations are used to calculate the real and imaginary parts of the complex dielectric constant. A very sensitive heating and cooling technique is used to study the dielectric behavior of these crystals at various temperatures. Debye's theory is used to calculate the relaxation times of these crystals.

Supported by a grant from Grants and Research Funding Committee at Southeast Missouri State University.

8:36

**I11 4 Quantized Magnetic Flux in Atomic Systems.** R.L. COLLINS, *retired*, HCOI Box 106C, Rockport, TX 78382 -- Magnetic flux within a superconducting ring is quantized in units of  $\Phi = h/2e$ . (1,2) This same flux quantum also plays a role within atomic systems. An oscillating charge "q" creates, about itself, an encircling and transient magnetic field. The Schrodinger equation requires correction of the  $\langle p \rangle$  operator,  $-i(\hbar/2\pi)\nabla$  becoming  $-i(\hbar/2\pi)\nabla - qA$  (where A is the vector potential). Following Feynman (3), a wave function written as  $\Psi(r) = [\rho(r)]^{1/2} \exp[i\theta(r)]$  leads to a current density  $J = (\hbar/2\pi m)(\nabla\theta - (2\pi q/\hbar)A)\rho$  or  $mv = (\hbar/2\pi)\nabla\theta - qA$ . On integrating this last equation along the displacement between turning points of the motion, the magnetic flux  $\Phi$  is readily obtained. The first term is

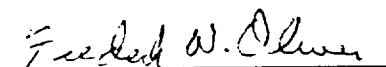
Abstract Submittal  
for the March 1996 Meeting  
of The American Physical Society  
18-22 March 1996

Sorting Category: 16. (b)

A Mossbauer Study of the Effects of Neutron Irradiation on a High Temperature Superconductor, F. W. OLIVER, E. HOFFMAN, D. SEIFU, E. HAMMOND, F. PIERRE, Z. KUREISHY, Morgan State Univ., Balto., MD, J. HOWARD, Hofstra University, Hempstead, N.Y., C. WYNTER, Nassau Community College, Nassau, N.Y. It has been found that neutron irradiation of high temperature superconductors change properties of the material<sup>1,2</sup>. We report on a Mossbauer investigation of neutron irradiated  $\text{EuBa}_2\text{Cu}_3\text{O}_x$  using the 21.53 keV transition of  $^{151}\text{Eu}$ . A sample was irradiated with approximately  $3.5 \times 10^{16}$  neutrons and a comparison made of the Mossbauer parameters for the irradiated and non-irradiated samples. Experimental results showed no difference between line-widths for this level of radiation but a measurable effect was seen for the isomer shift. A discussion of the isomer shift will be reported and compared with previous results found on irradiated low temperature superconductors.

1. B. Roas, B. Hensel, G. Saemann-Ischenko, and L. Schultz, Appl. Phys. Lett., 54(11), (March, 1989) p.1051.
2. J.-W. Lee, H.S. Lessure, D.E. Laughlin, M.E. McHenry, and S. G. Sankar, J. O. Willis, J.R. Cost, and M. Maley, Appl. Phys. Lett. 57(20) (November, 1990) p.2150.

Supported by NASA - NAG 5-2375



Frederick W. Oliver

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(X) Prefer Poster Session

## **APPENDIX B - SOFTWARE DEVELOPMENT**

```

%                               MOSS.m
%       This is a matlab version of parabola-lorentzian
%       least-squares analysis of Mossbauer data.
%
%

clear('L','M','aa','bb','chisq','count','delta','ee','ff','gama','gg','hh','i','il','k','k1','k2','k3','k4','mm','n1','n2','n3','nd','nn','pea
k','pp','qq','qqsq','tt','width','x','xmpps','xp','xpsq','xsq','y','ymax','ymin','yt','zz')

%#544    FE Foil

nd = 480;

L = 4;

bb(1) = 9.10 ; bb(2) = 8.41; bb(3) = 8.60; bb(4) = 8.73;

pp(1) = 86.73; pp(2) = 204.86; pp(3) = 301.72; pp(4) = 415.77;

M = zeros(48,10);

M = [ 48 X 10    ];

x=1:1:nd;

%y = zeros(nd);

y = reshape(M',1,480);

chisq=1;

ymin = y(1);
ymax = y(1);
for i=2:nd;
if y(i)<ymin
    ymin=y(i);
end
if y(i)>ymax
    ymax=y(i);
end
end

yminbs = ymin;
ymaxbs = ymax;

y = (y - ymin)./(ymax - ymin);
x = (x - 1)./(nd-1.);

pp = (pp - 1.)/(nd-1.)
bb = bb/(nd-1.)

hh = 1./(bb.^2)

```

```

count = 1

while (count) < 14

count = count + 1

for i=1:nd;
for k=1:L;
xp(k,i)=x(i)-pp(k);
xpsq(k,i)=xp(k,i).^2;
qq(k,i)=1+hh(k).*xp(k,i).^2;
qqsq(k,i)=qq(k,i).^2;
end
end

%tt = zeros(3+3*L,nd);
for il=1:nd;
for k1=0:L-1;
tt(1+3*k1,il)=1./qq(1+k1,il);
tt(2+3*k1,il)=xp(1+k1,il)./qqsq(1+k1,il);
tt(3+3*k1,il)=xpsq(1+k1,il)./qqsq(1+k1,il);
end
end
for il=1:nd;
tt(4+3*(L-1),il)= 1;
tt(5+3*(L-1),il)= x(il);
tt(6+3*(L-1),il)= x(il).^2;
end

mm = zeros(3*L+3,3*L+3);
for n1=1:3*L+3;
for n2=1:3*L+3;

mm(n1,n2) = sum(tt(n2,:).*tt(n1,:));

end
end

%nn = zeros(3*L+3,1);
for n3=1:3*L+3;

nn(n3,1)=sum(y.*tt(n3,:));

end
%det(mm)
zz = inv(mm)*nn;

for k2=1:L;
aa(k2) = zz(1+3.*(k2-1));
gama(k2) = zz(2+3.*(k2-1))/(2.*aa(k2).*hh(k2));
delta(k2) =-zz(3+3.*(k2-1))/aa(k2);
end
ee = zz(4+3*(L-1));
ff = zz(5+3*(L-1));

```

```

gg = zz(6+3*(L-1));

for k3=1:L;
hh(k3) = hh(k3) + delta(k3);
pp(k3) = pp(k3) + gama(k3);
end
for i=1:nd;
xsq(i) = x(i).^2;
for k4=1:L;
xmpps(k4,i) = (x(i) - pp(k4)).^2;
end
end

yt=(aa(1,1)./(1. + hh(1,1).*xmpps(1,:))) + (aa(1,2)./(1. + hh(1,2).*xmpps(2,:))) + (aa(1,3)./(1. +
hh(1,3).*xmpps(3,:))) + (aa(1,4)./(1. + hh(1,4).*xmpps(4,:))) + ee + ff.*x + gg.*xsq;

chisq = sum((y - yt).^2)./(nd-L)

yp=ee + ff.*x + gg.*xsq;
xpmin = - ff./(2.*gg);
xpminsq = xpmin.^2;
ypmin = ee + ff.*xpmin + gg.*xpminsq;

if (count) <=-1
y = y - yp + ypmin;
break
end
end

delta
gama
pp
hh
bb=1./sqrt(hh)
baseline = ee + ff.*xpmin + gg.*xpminsq

width = bb.*(nd-1.)
peak = pp.*(nd-1.) + 1.
cal544 = 2.245 ./(((peak(2)-peak(1)))+(peak(4)-peak(3)))./2.)

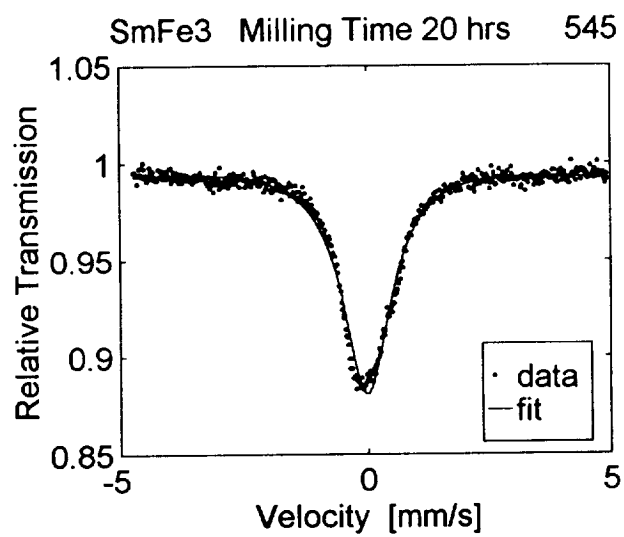
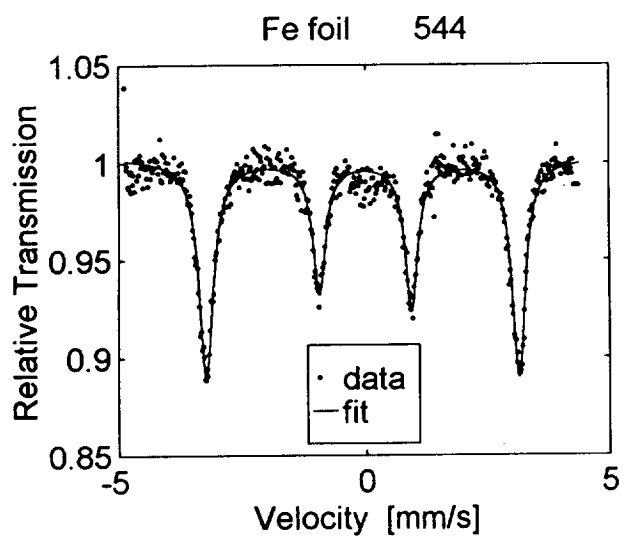
c544 = (peak(2) + peak(3))./2.
LW544 = bb.*(nd-1.).*cal544

x = (x - c544./nd).*cal544.*(nd-1.);
y = (y + yminbs./(ymaxbs - yminbs))./(baseline + yminbs./(ymaxbs - yminbs));
yt = (yt+ yminbs./(ymaxbs - yminbs))./(baseline + yminbs./(ymaxbs - yminbs));

subplot(2,1,1)
plot(x,y,'o',x,yt);
legend('data','fit')
title('Fe foil 544')
xlabel('Velocity [mm/s]')
ylabel('Relative Transmission')
print('plot.ps')

```





```
C
C THIS CODE GENERATES A LEAST SQUARES QUADRATIC FIT OF THE PARABOLA
C THAT APPEARS IN THE MOSSBAUER SPECTRUM WHICH ARISES DUE TO THE
C CHANGING SOLID ANGLE THE DETECTOR SEES BECAUSE OF THE MOTION OF
C THE SOURCE AND STRIPS IT OFF THE SPECTRUM. THIS PROCEDURE WILL
C ACCELERATE THE CONVERGENCE OF THE LORENTZIAN FITTING CODE.
C
C D.SEIFU , MORGAN STATE UNIVERSITY SUMMER OF 1995
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C IMPLICIT REAL*8 (A-H,O-Z)
C PARAMETER (N=3,NA=512,NB=46,NL=6,NPR=3*NL+1,NF=13)
C DIMENSION A(N,N),INDX(N),B(N),D(N,N),U(N,N),V(N),q(N)
C DIMENSION X(NA),Y(NA),YP(NA),DY(NA),YMP(NA)
C DIMENSION IBAD(NB)
C DIMENSION M(NF),FF(NPR)
C CHARACTER*80 FIL1,FIL2,FIL3,AA,BB
C
C WRITE(6,*) 'PLEASE INPUT THE NAME OF THE INPUT FILE.'
C WRITE(6,*)'NOTE THAT THE INPUT FILE SHOULD HAVE A .DAT EXTENSION.'
C READ(5,'(A80)') FIL1
C WRITE(6,*) 'PLEASE INPUT A NAME FOR A FILE LISTING X,Y AND YP.'
C READ(5,'(A80)') FIL2
C
C WRITE(6,*) 'PLEASE INPUT A NAME FOR THE OUTPUT FILE.'
C READ(5,'(A80)') FIL3
C WRITE(6,*) ' THE OUTPUTS WILL IN THE FILE NAMES YOU SPECIFIED WITH
> AN EXTENSION .DAT
> '
C
C WRITE(6,*) 'INPUT THE NO. OF CHANNELS TO BE OMITED ON THE LEFT
> SIDE OF THE MINIMA WHEN CONSTRUCTING THE PARABOLA.'
C READ(5,*) IDL
C WRITE(6,*) 'INPUT THE NO. OF CHANNELS TO BE OMITTED ON THE RIGHT
> SIDE OF THE MINIMA WHEN CONTRUCTING THE PARABOLA.'
C READ(5,*) IDR
C WRITE(6,*) 'IF THE LIST OF BAD DATA IS AT THE TOP OF THE DATA
> ENTER 1 ELSE ENTER 2.'
C READ(5,*) LBPT
C
C OPEN(UNIT=8,FILE= FIL1,STATUS='OLD')
C OPEN(UNIT=6,FILE= FIL2,STATUS='NEW')
C OPEN(UNIT=10,FILE= FIL3,STATUS='NEW')
C
C READ(8,'(30I5)') IBAD
C READ(8,'(////f)')
C
C READ(8,'(A80)') AA
C READ(8,'(A80)') BB
C READ(8,'(13I5,f10.0)') M,F
C READ(8,'(7f10.2)') FF
C
```

```

      IF(LBPT.EQ.1) THEN
      READ(8,'(14I5)') IBAD
      READ(8,'(10F7.0)')Y  !read in the values of y from file data.dat
      ELSE
      READ(8,'(10F7.0)')Y
      READ(8,'(14I5)') IBAD
      ENDIF
C
111 ND = M(1)
    NBP= M(2)
C
    WRITE(6,*)'ND =' ,ND,'NBP =' ,NBP
    WRITE(6,*) IBAD
C
    DO 1 I=1,ND
      X(I) = REAL(I)  !set up the value of x (velocity)
C    IF( Y(I).EQ.0.) THEN
C    Y(I) = (Y(I-1) + Y(I+1))/2.
C    ENDIF
1    CONTINUE
C
    YMIN=Y(15)
    DO 2 J=2,ND
    DO 23 I=1,NBP
      IF ( J.EQ.IBAD(I)) GOTO 2
23  CONTINUE
      IF( YMIN.GT.Y(J)) THEN  !search for the minimum value of y
      YMIN = Y(J)
      JMIN = J
      ENDIF
2    CONTINUE
C
    YMAX=Y(1)
    DO 21 J=2,ND
      IF( YMAX.LT.Y(J)) THEN  !search for the maximum value of y
      YMAX = Y(J)
      JMAX = J
      ENDIF
21  CONTINUE
C
    WRITE(6,*) 'YMIN=',YMIN,'YMAX=',YMAX
    WRITE(6,*) 'XMIN=',X(JMIN),'JMIN=',JMIN
C
    DO 22 I=1,ND
      Y(I)=(Y(I) - YMIN)/(YMAX-YMIN)  !scaling y to be bwn 0 and 1.
C    X(I)= X(I)/(REAL(ND))
22  CONTINUE
C
    H=YMAX-YMIN
C
    SYXSQ = 0.
    SXF  = 0.
    SXC  = 0.
    SXS  = 0.  !initialize the sums used in least squares fit.

```

```

SYX = 0.
SX = 0.
SY = 0.
C
DO 3 K=1,JMIN-IDL
DO 31 KK=1,NBP
IF (K.EQ.IBAD(KK)) GOTO 3
31 CONTINUE
SYXSQ = SYXSQ + Y(K)*(X(K)**2)
SXF = SXF + X(K)**4
SXC = SXC + X(K)**3
SXS = SXS + X(K)**2 ! calculate the value of the sums
SYX = SYX + Y(K)*X(K) ! used in the least squares fit.
SX = SX + X(K)
SY = SY + Y(K)
3 CONTINUE
C
DO 4 K=JMIN+IDR,ND
DO 41 KK=1,NBP
IF (K.EQ.IBAD(KK)) GOTO 4
41 CONTINUE
SYXSQ = SYXSQ + Y(K)*(X(K)**2)
SXF = SXF + X(K)**4
SXC = SXC + X(K)**3
SXS = SXS + X(K)**2
SYX = SYX + Y(K)*X(K)
SX = SX + X(K)
SY = SY + Y(K)
4 CONTINUE
C
ICB = 0
C
DO 45 I=1,JMIN-IDL
DO 46 II=1,NBP
IF(I.EQ.IBAD(II)) ICB=ICB + 1
46 CONTINUE
45 CONTINUE
C
DO 47 I=JMIN+IDR,ND
DO 48 II=1,NBP
IF(I.EQ.IBAD(II)) ICB=ICB + 1
48 CONTINUE
47 CONTINUE
C
wt = REAL(ND-IDL-IDR-ICB)
C
WRITE(6,*) 'wt = ',wt
WRITE(6,*) 'ICB = ',ICB
C
A(3,1)= SXF/ wt
A(3,2)= SXC/ wt ! set up a 3X3 matrix
A(3,3)= SXS/ wt ! to solve for the coeff
A(2,1)= SXC/ wt ! of the parabola
A(2,2)= SXS/ wt ! y=v1*x^2 + v2*x + v3

```

```

A(2,3)= SX / wt
A(1,1)= SXS/ wt
A(1,2)= SX / wt
A(1,3)= 1.
C
B(3)= SYXSQ/ wt
B(2)= SYX/ wt          ! the right side of the equation
B(1)= SY/ wt           !   Av = B
C
DO 88 I=1,N
DO 77 J=1,N
WRITE(6,*)'A',I,J,'=',A(I,J)
77 CONTINUE
WRITE(6,*)'B',I,'=',B(I)
88 CONTINUE
C
D(1,1) = 1.
D(2,2) = 1.
D(3,3) = 1.
C
U(1,1) = A(1,1)
U(1,2) = A(1,2)          ! STARTING THE LU DECOMPOSITION.
U(1,3) = A(1,3)
C
D(2,1) = A(2,1)/A(1,1)
U(2,2) = A(2,2) - D(2,1)*U(1,2)
U(2,3) = A(2,3) - D(2,1)*U(1,3)
C
D(3,1) = A(3,1)/U(1,1)
D(3,2) = (A(3,2) - (D(3,1)*U(1,2)))/U(2,2)
U(3,3) = A(3,3) - D(3,1)*U(1,3) - D(3,2)*U(2,3)
C
Q(1) = B(1)/D(1,1)          ! THE LU BACK SUBSTITUTION.
Q(2) = (B(2) - (D(2,1)*Q(1)))/D(2,2)
Q(3) = (B(3) - (D(3,1)*Q(1)) - (D(3,2)*Q(2)))/D(3,3)
C
V(3) = Q(3)/U(3,3)
V(2) = (Q(2) - (U(2,3)*V(3)))/U(2,2) ! COEFFICIENTS OF THE PARAB.
V(1) = (Q(1) - (U(1,2)*V(2)) - (U(1,3)*V(3)))/U(1,1)
C
V(3) = V(3)*(YMAX-YMIN) + YMIN
V(2) = V(2)*(YMAX-YMIN)          ! RESCALING THE COEFFICIENTS.
V(1) = V(1)*(YMAX-YMIN)
C
DO 5 I=1,ND
X(I) = REAL(I)
5 CONTINUE
C
WRITE(6,'(///)')
WRITE(6,*)'THE EQUATION OF THE PARABOLA REMOVED FROM THE DATA IS'
WRITE(6,'(//)')
WRITE(6,*) 'Y=',V(1),'X^2+',V(2),'X+',V(3)
C
DO 6 J=1,ND

```

```

C   X(J) = X(J)*(REAL(ND-1)) + 1.
    YP(J) = V(1)*(X(J)**2) + V(2)*X(J) + V(3) !eqn of the parabola
    DY(J) = Y(J) - YP(J)                  ! diff with the data
6   CONTINUE
C
    write(6,*)'JMIN=',JMIN,'X(JMIN)=',X(JMIN),
>    'Y(JMIN)=',Y(JMIN),'YP(JMIN)=',YP(JMIN)
    write(6,*)'JMAX=',JMAX,'X(JMAX)=',X(JMAX),
>    'Y(JMAX)=',Y(JMAX),'YP(JMAX)=',YP(JMAX)
    write(6,*) 'ymin =',ymin,'ymax =',ymax
C   write(6,'(10F8.0)') DY
C
    YPMIN=YP(1)
    DO 7 J=2,ND
    IF( YPMIN.GT.YP(J)) THEN  ! search for the minima of the parabola
    YPMIN = YP(J)
    JPMIN = J
    ENDIF
7   CONTINUE
C
    YPMAX=YP(1)
    DO 71 J=2,ND
    IF( YPMAX.LT.YP(J)) THEN  ! search for the maxima of the parabola
    YPMAX = YP(J)
    JPMAX = J
    ENDIF
71  CONTINUE
C
C   if (ypmin.lt.ymin) ymin = ypmin  ! set ymin to the lowest minima
C   if (ypmax.gt.ymax) ymax = ymax  ! set ymax to the highest maxima
    H = ymax - ymin
C
    DO 8 I=1,ND
    Y(I) = Y(I)*(YMAX - YMIN) + YMIN
    YMP(I)= y(i)-yp(i)+YPMIN
8   CONTINUE
C
C   DO 99 I=1,ND
C   DO 92 II=1,NBP
C   IF( I.EQ.IBAD(II)) YMP(I) = (YMP(I-1) + YMP(I+1))/2.
C 92  CONTINUE
C 99  CONTINUE
C
    WRITE(10,'(A80)') AA
    WRITE(10,'(A80)') BB
    WRITE(10,'(13I5,f10.0)') M,F
    WRITE(10,'(7F10.2)') FF
    WRITE(10,'(10F7.0)') YMP
    WRITE(10,'(14I5)')IBAD
C
    DO 100 I=1,ND
    WRITE(6,'(F7.0,3X,F7.0,3X,F7.0,3X,F10.0)') X(I),Y(I),YP(I),YMP(I)
100  CONTINUE
    END

```

The following software represents a modification of the computer code provided by Austin science into one that gives a final plot of the Moessbauer data which is ready for presentation.

```

10 REM                                MOSSPLOT.BAS
15 COLOR 1, 11
20 CLS : KEY OFF
22 LOCATE 2, 1
25 PRINT "Adapted from a program by R.L. Collins, Austin
Science Associates, Inc.,"
30 PRINT "                                Austin TX 78745"
40 PRINT " Fall, 1995, version by E.J. Hoffman, Morgan
State University Physics Dept."
50 PRINT : PRINT : PRINT : PRINT : PRINT
60 PRINT "                                Welcome to":
PRINT
65 PRINT "                                M O S S P L O
T": PRINT
66 GOSUB 10050: REM Delay
67 DIM Y(515): DIM G(515): DIM M(515): DIM V(1515)
68 FQ$ = "FQ": REM so that NEWFQ$ <> FQ$

70 CLS
72 ON KEY(10) GOSUB 10100: KEY(10) ON: REM Setting F10 for
returning to the menu at any time
73 PR = 0
74 ON KEY(5) GOSUB 10160: KEY(5) ON: REM Setting F5 for
use of the line printer

75 LOCATE 10, 12: PRINT "IF YOU WISH THE LINE PRINTER TO
RECORD THE OPERATION,"
76 PRINT: PRINT "                                PRESS
FUNCTION KEY F5"
77 BEEP: GOSUB 10050: GOSUB 10050: CLS

78 LOCATE 25, 8
79 PRINT "TO RETURN TO THE MENU AT ANY TIME PRESS FUNCTION
KEY F10 (Enter)"

80 NUTEMS$ = "": NEWFILE$ = "": DAT$ = "": BOX$ = ""
82 LOCATE 1, 35
84 PRINT "MENU": PRINT
85 PRINT "    1) Plot a theoretical curve from parameters
given by the"
86 PRINT "                MOSS curve-fitting program (on the
VAX)": PRINT
90 PRINT "    2) Print out the data from 512-channel
*.spm files created"
91 PRINT "                by the ASA-modified The Nucleus PCA":
PRINT
95 PRINT "    3) Create a .INP file for input into the
MOSS program": PRINT
100 PRINT "    4) For a *.spm file, calculate velocity
from interferometer data:"
101 PRINT "                plot counts versus velocity"
102 PRINT "    4') For a *.spm file run without the
interferometer,"
103 PRINT "                plot counts versus channel number":
PRINT
105 PRINT "    5) Overplot a fitted curve from parameters
given by the MOSS program": PRINT
107 PRINT "    6) Plot data points and overplot the
fitted curve from a .DAT"
108 PRINT "                file downloaded from the VAX": PRINT
110 PRINT "    7) Exit MossPlot"
120 PRINT : INPUT "                Enter your choice from the
menu by number: ", NUTEMS$
124 ITEM$ = NUTEMS$
125 ON ERROR GOTO 10300
126 IF ITEM$ <> "7" AND PR=1 THEN LPRINT : LPRINT "
"; DATE$; "    "; TIME$; "    MOSSPLOT Menu Choice: ";
ITEM$: LPRINT
127 ON ERROR GOTO 0

129 PNTS% = 512: REM Item 6 may alter this
130 IF ITEM$ = "1" THEN CLS : GOTO 6000
140 IF ITEM$ = "2" THEN CLS : GOTO 1000
150 IF ITEM$ = "3" THEN CLS : GOTO 3000
155 IF ITEM$ = "4" THEN VELSTD$ = " by interferometry"
160 IF ITEM$ = "4" OR ITEM$ = "4'" THEN CLS : GOTO 6000
170 IF ITEM$ = "5" THEN CLS : BOX$ = "DRAWN": GOTO 6180

```

```

180 IF ITEM$ = "6" THEN CLS : GOTO 2000
190 IF ITEM$ = "7" THEN CLS : GOTO 600
200 GOTO 130

```

```

600 CLS
605 LOCATE 25, 2
610 INPUT "Exit MOSSPLOT (yes, no)": EX$
620 IF EX$ = "Y" OR EX$ = "y" THEN COLOR 7,0: CLS: END
630 GOTO 70

700 REM Loading a *.spm file
702 IF FS$ = "" THEN GOTO 720
708 PRINT "                Do you want to process "; FS$; " again
(y, n)?"
709 INPUT "                                ", REFILE$
710 IF REFILE$ = "Y" OR REFILE$ = "y" THEN RETURN
720 DIM X(4000): PRINT : 'PRINT: PRINT
730 INPUT "Name of .spm file (you may type it without the
.spn extension): ", NEWFILE$
732 PRINT : PRINT
740 DGT = 1: REM Initializing at the first digit
745 WHILE CH$ <> CHR$(46) AND DGT < (LEN(NEWFILE$) + 2):
REM Up to the dot if there is one
750     CH$ = MID$(NEWFILE$, DGT, 1): REM Filename
character
755     DGT = DGT + 1
760 WEND
762 NEWFQ$ = LEFT$(NEWFILE$, DGT-2): REM Filename without
dot or extension
764 IF NEWFQ$ = FQ$ THEN RETURN
766 FQ$ = NEWFQ$
765 FS$ = FQ$ + ".spm"
767 ON ERROR GOTO 10175
768 REM error 53
770 OPEN FS$ FOR RANDOM AS #1 LEN = 64
772 ON ERROR GOTO 0
775 FIELD #1, 64 AS A$
780 GET #1, 1
785 FOR I = 9 TO 40
790     GET #1, I
800     FOR J = 1 TO 64
810         K = 64 * (I - 1) + J
820         B$ = MID$(A$, J, 1)
830         X(K) = ASC(B$)
840     NEXT J
845 NEXT I
850 FOR I = 1 TO PNTS%
860     N = 504 + 4 * I
870     Y(I) = X(N + 1) + 256 * (X(N + 2) + 256 * X(N +
3))
880 NEXT I
883 CLOSE #1
885 FOR I = 1 TO 512
886     IF Y(I) <> 0 GOTO 890
887 NEXT I
888 ERROR 53
889 ON ERROR GOTO 0
890 IF PR=1 THEN LPRINT : LPRINT "Data File Loaded:
"; FS$: LPRINT
900 RETURN

```

```

1000 REM Raw data printout routine
1010 GOSUB 700
1440 FOR I = 1 TO 512 STEP 8
1449 ON ERROR GOTO 10300
1450     LPRINT USING "#####"; I;
1451 ON ERROR GOTO 0
1460     FOR J = 0 TO 7
1465         DIM A(512)
1470         A(J) = Y(I + J)
1480         LPRINT USING "##### "; A(J);
1490         IF J = 7 THEN LPRINT ""
1500     NEXT J
1510 NEXT I
1520 GOTO 70

```

```

2000 REM Processing a *.DAT file

```



```

2005 INPUT "Name of source (downloaded *.DAT) file: ",
DAT$
2010 PRINT
2015 FS$ = DAT$
2018 ON ERROR GOTO 10200
2020 OPEN DAT$ FOR INPUT AS #2
2021 ON ERROR GOTO 0
2025 ENDJUNK$ = "AL DATA": REM For experimental points
2030 GOSUB 2800
2035 GOSUB 2700: REM For baseline
2055 PRINT: PRINT "Is this a europium run or an iron run?
(Answer "; CHR$(34); "E"; CHR$(34); " or "; CHR$(34); "F";
CHR$(34); ")"
2057 INPUT " ", EF$
2060 IF EF$ <> "E" AND EF$ <> "e" AND EF$ <> "F" AND EF$
<> "f" THEN GOTO 12900
2070 IF EF$ = "F" OR EF$ = "f" THEN VELSTD$ = " relative
to iron": STDEUS$ = "": GOTO 2100
2071 VELSTD$ = " relative to europium fluoride"
2075 GOTO 12000

```

```

2100 IF STDFE$ <> "" THEN INPUT "Want to use the same Fe
standard run for calibration"; REPEATSTD$
2103 IF REPEATSTD$ = "Y" OR REPEATSTD$ = "y" THEN GOTO
2111
2105 PRINT : PRINT "Name of Fe standard run for
calibration"
2110 PRINT " ("; CHR$(34); "Enter"; CHR$(34); : INPUT
"if no calibration desired):", STDFE$
2111 PRINT : PRINT
2130 IF STDFE$ = "" THEN GOTO 2410
2135 ITEM$ = "CAL6"
2136 IF REPEATSTD$ = "Y" OR REPEATSTD$ = "y" THEN PRINT :
GOTO 2287
2137 DIM PK(10)
2140 READPK$ = STDFE$: GOSUB 2600
2150 CALIBRFE = PEAK
2155 IF VELSTD$ = " relative to iron" AND STDFE$ <> ""
THEN FS$ = FS$ + ", calibrated using " + STDFE$
2160 IF STDEUS$ <> "" THEN FS$ = FS$ + ", calibrated using
" + STDEUS$ + " and " + STDFE$
2170 IF PR=1 THEN LPRINT: LPRINT "Data File: "; FS$:
LPRINT
2180 IF STDEUS$ <> "" AND PR=1 THEN LPRINT "Peak of the Eu
standard run is at channel "; CALIBREU

```

```

2209 REM hyperfine splitting calculation follows
2210 IF N = 6 THEN HFS = ((PK(6) - PK(4)) + (PK(3) -
PK(1))) / 4
2215 IF N = 4 THEN HFS = ((PK(5) - PK(4)) + (PK(3) -
PK(2))) / 2
2220 PRINT : PRINT "Peak of the Fe standard run = the
average of "; N; " positions = Channel "; CALIBRFE
2225 IF PR=1 THEN LPRINT : LPRINT "Peak of the Fe standard
run = the average of "; N; " positions = Channel ";
CALIBRFE
2230 PRINT : PRINT "The hyperfine splitting = the average
of the spacings"
2235 PRINT " between peaks 1-2, 2-3, 4-5, and 5-6
= "; HFS; " channels"
2240 IF PR=1 THEN LPRINT : LPRINT "The hyperfine splitting
= the average of the spacings"
2245 IF PR=1 THEN LPRINT " between peaks 1-2, 2-3,
4-5, and 5-6 = "; HFS; " channels"
2255 HFSSTD = 2.245: REM Standard HFS in mm/s
2260 B = HFSSTD / HFS: REM Slope of the velocity vs.
channel no. curve
2261 PRINT : PRINT "The calibration constant = "; HFSSTD;
"/"; HFS; " = "; B; " (mm/s)/channel"
2262 IF PR=1 THEN LPRINT : LPRINT "The calibration
constant = "; HFSSTD; "/"; HFS; " = "; B; "
(mm/s)/channel"
2263 PRINT : IF PR=1 THEN LPRINT : LPRINT
2265 IF EF$ = "E" OR EF$ = "e" THEN ISSTD = CALIBREU
2267 IF EF$ = "F" OR EF$ = "f" THEN ISSTD = CALIBRFE
2270 A = -B * ISSTD: C = 0: REM V = A + BX + CX^2;

```

```

linearity assumed here
2275 REM To get the isomer shift for the sample
2282 READPK$ = DAT$
2285 IF EF$ = "E" OR EF$ = "e" THEN GOSUB 12600
2287 IF EF$ = "F" OR EF$ = "f" THEN GOSUB 2600
2290 IS = B*(PEAK - ISSTD)
2295 PRINT: PRINT "Isomer shift"; VELSTD$; " for "
2296 PRINT " "; FS$; " "
2297 PRINT: PRINT " "; B; "X("; PEAK; " - "; ISSTD; ")
= "; IS; " mm/s"
2300 IF PR=1 THEN LPRINT: LPRINT "Isomer shift"; VELSTD$;
" for "; FS$; " "
2301 IF PR=1 THEN LPRINT " "; B; "X("; PEAK; " - ";
ISSTD; ") = "; IS; " mm/s"

```

```

2310 PRINT: PRINT " Do you want an extra
x and y scale,"
2320 PRINT " for channel number and for
counts,"
2330 PRINT " (answer "; CHR$(34); "n";
CHR$(34); " for a plot being"
2340 PRINT " prepared for
publication)"
2350 INPUT " (y, n); SCALE$
2360 IF SCALE$ = "n" OR SCALE$ = "N" THEN ITEM$ = "PUB6"
2365 IF YS = 0 OR SCALE$ = "y" OR SCALE$ = "Y" THEN GOTO
2410
2370 PRINT : PRINT " Would you like to re-use
the same"
2380 PRINT " Absorption axis scaling as in
the"
2390 PRINT " last plot, rather than an
auto-"
2400 INPUT " ically-maximized scale (y,
n); REPEATSC$
2405 PRINT : PRINT
2410 GOSUB 6029

```

```

2500 OPEN DAT$ FOR INPUT AS #2
2505 ENDJUNK$ = "CAL FIT": REM For theoretical points
2510 GOSUB 2800
2520 CLOSE #2
2590 ITEM$ = "5": GOTO 6183

```

```

2600 REM Reading peak positions and calculating average
2603 ON ERROR GOTO 10225
2605 OPEN READPK$ FOR INPUT AS #3
2606 ON ERROR GOTO 0
2610 JUNK$ = ""
2615 WHILE RIGHT$(JUNK$, 6) <> "TO 0.5"
2620 LINE INPUT #3, JUNK$
2621 WEND
2623 INPUT #3, JUNK
2624 INPUT #3, JUNK
2625 INPUT #3, JUNK
2626 INPUT #3, JUNK
2627 INPUT #3, JUNK
2628 INPUT #3, JUNK
2630 INPUT #3, NRPARAMS
2635 N = (NRPARAMS - 1)/3
2636 IF N <> 6 AND N <> 4 THEN GOTO 10325
2640 JUNK = 0
2645 WHILE JUNK <> (1 + 2*N + 1)
2650 INPUT #3, JUNK
2655 WEND
2680 FOR I = (4 - (N/2)) TO (3 + (N/2))
2683 INPUT #3, PK(I): INPUT #3, JUNK: INPUT #3, JUNK
2685 NEXT I
2686 CLOSE #3
2687 PEAK = 0
2688 FOR I = (4 - (N/2)) TO (3 + (N/2))
2689 PEAK = PEAK + PK(I)
2690 NEXT I
2691 PEAK = PEAK / N: REM Isomer shift = avg. of N
positions
2699 RETURN

```

```

2700 REM Reading the converged baseline value
2710 JUNK$ = ""
2720 WHILE RIGHT$(JUNK$, 9) <> "DEVIATION"
2730   LINE INPUT #2, JUNK$
2740 WEND
2750 INPUT #2, JUNK%
2770 INPUT #2, B3
2790 RETURN

2800 REM Read-in loops
2810 JUNK$ = ""
2820 WHILE RIGHT$(JUNK$, 7) <> ENDJUNK$
2830   LINE INPUT #2, JUNK$
2840 WEND
2850 LINE INPUT #2, JUNK$ : 'print " JUNK$ = "; JUNK$
2860 LINE INPUT #2, JUNK$ : 'print " JUNK$ = "; JUNK$
2870 I = 1: Y(0) = 1
2880 'WHILE (Y(I) <> 0) OR (Y(I-1) <> 0)
2885 FOR I = 1 TO PNTS%
2890   INPUT #2, Y(I)
2895   'print: print "      I = "; I; "      Y(I) = ";
Y(I); rem ; "      Y(I-1) = "; Y(I-1)
2896   'gosub 10050: 'gosub 10050: GOSUB 10050: GOSUB
10050
2898   'if (y(i)=0) and (y(i-1)=0) goto 2920
2900   'I = I + 1
2910 next i: 'WEND
2911 'gosub 10050
2915   'print: print "      I = "; I; "      Y(I) = ";
Y(I); "      Y(I-1) = "; Y(I-1)
2920 'PNTS% = I - 3
2925   'print: print "      PNTS% = "; PNTS%
2930 RETURN

3000 REM To save the data as a .INP file suitable for
input into the MOSS program
3010 YADD% = 0: REM Assume 6-digit counts until line 3124
3020 GOSUB 700
3030 FR$ = FQ$ + ".INP": REM New filename is the same with
".INP" instead of ".spm"
3040 PRINT : PRINT : PRINT "      A file is being
saved suitable for input into the MOSS program."
3050 PRINT : PRINT "      The new
filename will be "; FR$
3052 IF P$ <> "" THEN GOTO 3700
3060 PRINT "Type any description you wish to add to the
filename (< 64 characters):"
3070 PRINT: INPUT " ", DESCR$
3080 PRINT : PRINT : INPUT "      How many lines in the
spectrum"; N
3090 PRINT: PRINT "      Enter estimated parameters (ENTER
for zero spacers)": GOSUB 5100
3100 OPEN FR$ FOR OUTPUT AS #1
3120 LSET EORF$ = CHR$(13) + CHR$(10): REM Carriage retn.
+ linefeed
3121 YIJ$ = STR$(Y(105)): REM Counts in channel 105 used
as a sample
3122 REM The next line strips the space added by STR$ from
the left
3123 YIJ$ = RIGHT$(YIJ$, LEN(YIJ$) - 1)
3124 IF LEN(YIJ$) = 7 THEN GOSUB 3500: REM For stripping
off the first 1

3140 PRINT #1, "1      (10F7.0)"
3145 PRINT #1, CHR$(35); FQ$; " "; DESCR$
3150 PRINT #1, USING "#####. "; PNTS%; (15 + INT((PNTS% -
5)/16)); 1; N; (3*N + 1); 0; 0; 0; 1; 1; 1; 0; 0; YADD%;
3155 PRINT #1, "."
3160 PRINT #1, USING "#####. "; B3;
3165 FOR I = 1 TO N
3167   AREA!(I) = -ABS(AREA!(I))
3170   PRINT #1, USING "#####. "; AREA!(I);
3173   IF (1+I) = 7 THEN PRINT #1, EORF$
3175 NEXT I

```

```

3182 FOR J = 1 TO N
3184   PRINT #1, USING "###. "; LW!(J);
3186   IF (1+N+J) = 7 OR (1+N+J) = 14 OR (1+N+J) = 21
THEN PRINT #1, EORF$
3188 NEXT J
3192 FOR K = 1 TO N
3194   PRINT #1, USING "###. "; NRG!(K);
3196   IF (1+(2*N)+K) = 7 OR (1+(2*N)+K) = 14 OR
(1+(2*N)+K) = 21 OR K = N THEN PRINT #1, EORF$
3198 NEXT K

```

```

3200 FOR I = 1 TO PNTS% STEP 10
3205   FOR J = 0 TO 9
3210     IF (I + J) > PNTS% GOTO 3300
3230     PRINT #1, USING "#####. "; Y(I + J);
3240     IF J = 9 THEN PRINT #1, EORF$
3250   NEXT J
3260 NEXT I

```

```

3300 REM The following are NBAD(I), the channel numbers to
be omitted by MOSS
3310 PRINT #1, EORF$
3320 FOR I = 1 TO 14: REM Discarding the 1st 14
points(non-data)
3340   PRINT #1, USING "#####. "; I;
3350 NEXT I
3360 PRINT #1, EORF$
3365 K = 0: REM Counter for 14-digit lines
3370 FOR I = 16 TO PNTS% STEP 16
3380   PRINT #1, USING "#####. "; I;
3385   K = K + 1
3390   IF INT(K/14) = (K/14) THEN PRINT #1, EORF$
3400 NEXT I

```

```

3470 CLOSE #1
3480 FS$ = ""
3490 GOSUB 10000
3495 GOTO 70

```

```

3500 REM Routine for handling 7-digit counts
3510 YADD% = 1
3540 FOR I = 1 TO 512
3550   YI$ = STR$(Y(I))
3560   REM The next line strips the space added by STR$
AND the 1 from the left
3570   YI$ = RIGHT$(YI$, LEN(YI$) - 2)
3580   Y(I) = VAL(YI$)
3590 NEXT I
3600 RETURN

```

```

3700 PRINT: PRINT "Would you like "; CHR$(34); P$;
CHR$(34)
3710 INPUT "      to be printed as a description in the
file"; PAGAIN$
3720 IF PAGAIN$ = "y" OR PAGAIN$ = "Y" THEN DESCR$ = P$:
GOTO 3080
3730 GOTO 3060

```

```

4000 REM Velocity formula calculation
4005 'PRINT "PROGRAM ASSUMES 512 CHANNELS, FLYBACK MODE"
4100 'PRINT "LASER MULTIPLEXES INTO EVERY 16TH CHANNEL"
4140 'PRINT "TIMING INFO. ASSUMED:"
4145 'PRINT "      CH 9, ZERO VEL. IN CH 264"
4150 'PRINT "IF NOT, CHANGE DATA IN LINE 4160."
4159 'PRINT: PRINT "Velocity formula calculation:"
4160 A7 = 9: A9 = 264
4170 N = 0: A0 = 0: A1 = 0: A2 = 0: A3 = 0: A4 = 0: A5 =
0: A6 = 0
4180 REM STARTING AND ENDING CH. NOS. ARE T1% AND T2%
4190 T1% = 96: T2% = 432: REM, 8/95, Setup B reliable only
in this range
4200 M1 = Y(9)
4240 B1 = 7.910248
4250 FOR X = T1% TO T2% STEP 16
4260   M = Y(X)
4300   M = M * B1 / M1

```

```

4310 IF X < A9 THEN 4330
4320 GOTO 4340
4330 M = -M
4340 N = N + 1
4350 A0 = A0 + X
4360 A1 = A1 + X * X
4370 A2 = A2 + M
4380 A3 = A3 + X * X * X
4390 A4 = A4 + X * M
4400 A5 = A5 + X * X * X * X
4410 A6 = A6 + X * X * M
4420 NEXT X
4430 REM NOW TO FIND PARAMETERS IN VEL(X)=A+BX+CXX
4440 D = N * (A1 * A5 - A3 * A3) - A0 * (A0 * A5 - A1 *
A3) + A1 * (A0 * A3 - A1 * A1)
4450 N1 = A2 * (A1 * A5 - A3 * A3) - A0 * (A4 * A5 - A3 *
A6) + A1 * (A4 * A3 - A1 * A6)
4460 N2 = N * (A4 * A5 - A3 * A6) - A2 * (A0 * A5 - A1 *
A3) + A1 * (A0 * A6 - A1 * A4)
4465 N3 = N * (A1 * A6 - A3 * A4) - A0 * (A0 * A6 - A1 *
A4) + A2 * (A0 * A3 - A1 * A1)
4470 A = N1 / D: B = N2 / D: C = N3 / D
4480 IF PR=1 THEN LPRINT "VEL(X)="; A; "+ "; B; "X+ "; C;
"X^2"
4481 IF PR=1 THEN LPRINT "          where X is channel
number"
4483 IF PR=1 THEN LPRINT : LPRINT
4484 PRINT "VEL(X)= "; A; "+ "; B; "X+ "; C; "X^2"
4485 PRINT "where X is channel number"
4487 PRINT : PRINT          NOTE THAT THE QUADRATIC
COEFFICIENT IS ": PRINT
4488 PRINT "          "; C: PRINT
4492 PRINT "          For the best linearity the quadratic
coefficient should vanish."
4494 PRINT "          Use the UltraLin program for easy
adjustment of the ultralinear control."
4500 RETURN: REM To line 6078

```

```

5000 REM Routine for calculating Y(X), the fitted curve
5001 CLS
5005 T1% = 5: T2% = 511
5010 PRINT : PRINT : INPUT "How many lines in the
spectrum"; N
5020 PI! = 4 * ATN(1): REM Pi = 4 X arctan(1)
5030 PRINT : PRINT "Enter values from the converged
curvefit: "
5040 DIM YY(3 * N): DIM BB(3 * N): DIM ZZ(3 * N): DIM GG(3
* N): DIM AA(3 * N, 6 * N)
5050 'DIM NRG!(N): DIM AREA!(N): DIM LW!(N)
5100 PRINT : PRINT : INPUT "Enter the baseline ", B3
5101 IF PR=1 THEN LPRINT : LPRINT "          Values
entered:"
5105 IF PR=1 THEN LPRINT : LPRINT "Baseline (counts): ";
B3
5110 PRINT : PRINT : PRINT "Enter the parameters for each
line:"
5111 FOR I = 1 TO N
5112 IF N = 1 THEN PRINT : GOTO 5120
5115 PRINT : PRINT "For Line No. "; I; ":"
5120 PRINT : INPUT "          Absolute value of area under
curve (channels X counts): ", AREA!(I)
5130 PRINT : INPUT "          Line width (channels): ",
LW!(I)
5140 PRINT : INPUT "          Position: Channel No. ",
NRG!(I)
5160 IF N = 1 THEN GOTO 5180
5170 IF PR=1 THEN LPRINT : LPRINT "          For Line No.
"; I
5180 IF PR=1 THEN LPRINT : LPRINT "          Absolute value
of area under curve"
5185 IF PR=1 THEN LPRINT "          (channels
X counts): ", AREA!(I)
5190 IF PR=1 THEN LPRINT "          Line width (channels):
", LW!(I)
5200 IF PR=1 THEN LPRINT "          Position: Channel No.

```

```

", NRG!(I)
5205 IF ITEM$="3" THEN GOTO 5250
5210 YY(N + I) = NRG!(I)
5230 YY(I) = AREA!(I) / (PI! * LW!(I)): REM Assumes
AREA! = PI x LW! x DEPTH OF DIP
5240 YY(2 * N + I) = (LW!(I)) / 2: REM Austin's program
uses half-width
5250 NEXT I
5255 IF ITEM$="3" THEN RETURN

```

```

5260 FOR X = T1% TO T2%: REM Initializing Y(X)
5280 Y(X) = 0
5290 NEXT X

```

```

5300 FOR X = T1% TO T2%
5330 FOR I = 1 TO N
5340 Y(X) = Y(X) + YY(I) / (1 + (X - YY(N + I)) * (X
- YY(N + I)) / (YY(2 * N + I) * YY(2 * N + I)))
5350 NEXT I
5360 Y(X) = B3 - Y(X)
5370 NEXT X

```

```

5380 RETURN

```

```

6000 REM PLOT ROUTINE FOR HP 7440A COLORPRO PLOTTER
6010 PRINT : PRINT : PRINT
6021 IF ITEM$ = "1" THEN CLS : PRINT "Enter a title
to be printed at the"
6022 IF ITEM$ = "1" THEN INPUT "upper left above the
plot: ", F$$: GOTO 6031
6025 GOSUB 700
6029 PRINT : PRINT " "; CHR$(34); F$$; CHR$(34);
6030 PRINT : PRINT "will be printed at the upper
left above the plot."
6031 PRINT : PRINT "Enter anything else you
wish to appear as "
6032 PRINT "a subtitle ("; CHR$(34);
"Enter"; CHR$(34); " for nothing else: "
6033 PRINT : INPUT " ", P$
6034 IF ITEM$ = "1" THEN PRINT " "; F$$:
GOSUB 5000
6035 IF ITEM$ = "CAL6" OR ITEM$ = "PUB6" THEN GOTO 6080
6037 IF ITEM$ = "1" OR ITEM$ = "6" OR ITEM$ = "4" THEN
GOTO 6090
6046 SOURCE$ = "Co-57": MATRIX$ = "Rh": P2 = .14
6047 PRINT : PRINT "NOTE: This program assumes a ";
SOURCE$; "source in a "; MATRIX$; " matrix:"
6048 PRINT "velocity offset = "; P2;
" mm/s"
6075 GOSUB 4000: REM For velocity formula
6080 FOR X = 1 TO 1200
6082 V(X) = A + B * X + C * X * X
6084 NEXT X
6085 P4 = INT(V(INT(.9 * (PNTS%))))
6086 IF P4 > 4 AND INT(P4 / 2) <> (P4 / 2) THEN P4 = P4 -
1
6087 IF P4 > 4 AND INT(P4 / 4) <> (P4 / 4) THEN P4 = P4 +
2
6088 IF P4 = 3 THEN P5 = 1 ELSE P5 = (P4) / 4: REM Max.
vel. and tic spacing
6090 PRINT : PRINT
6091 PRINT "LOAD BLANK SHEET OF PAPER, AND SET
SWITCH BOX TO "; CHR$(34); "A"; CHR$(34)
6095 GOSUB 10000: PRINT : 'PRINT : 'PRINT : PRINT
6160 PRINT : INPUT "IS PLOTTER READY (yes, no) "; AA$: REM
Plot routine for curve or points
6174 IF AA$ = "N" OR AA$ = "n" THEN CLS : GOTO 6090
6175 CLS : LOCATE 9, 30
6176 PRINT "PLOTING "; F$$
6180 IF ITEM$ = "5" THEN GOSUB 5000
6182 ON ERROR GOTO 10275
6183 OPEN "COM2:9600,S,7,1,RS,CS65535,DS,CD" FOR RANDOM AS
#1
6184 ON ERROR GOTO 0

```

```

6185 GOSUB 9000: REM For plotter setup codes
6186 IF ITEMS$ = "5" THEN GOTO 7000
6188 PRINT#1, "SP1";
6200 REM y axis scales
6205 T1% = 17
6210 IF ITEMS$ <> "1" AND ITEMS$ <> "6" AND ITEMS$ <> "CAL6"
AND ITEMS$ <> "PUB6" THEN GOSUB 11000
6220 IF ITEMS$ = "1" OR ITEMS$ = "6" OR ITEMS$ = "CAL6" OR
ITEMS$ = "PUB6" THEN MAXCNT = B3: GOSUB 11065

6290 REM For x axes
6295 IF ITEMS$ = "1" OR ITEMS$ = "4" OR ITEMS$ = "6" THEN
GOTO 6340
6300 P6 = -P4
6301 'print "At line 6301, P4 = "; P4; ", and P6 = ";
P6
6302 'while inkey$ = ""
6303 'wend
6321 F3 = V(PNTS%) - V(T1%): REM For scaling x axis
6322 REM F3 = B*(PNTS%-T1%) + C*(PNTS%^2-20^2): REM
Collins had F3 from 25 to PNTS%
6323 WHILE P6 <= P4: REM New x-axis velocity labelling
routine
6324 GOSUB 8600
6325 P6 = P6 + P5
6326 WEND: IF ITEMS$ = "PUB6" GOTO 6360
6327 'FOR X = T1% TO T2%: REM Collins' routine
6330 'IF (V(X) - P6) >= 0 THEN GOSUB 8900: REM x axis
labelling with velocity
6335 'NEXT X
6340 PNTS2% = PNTS% - (PNTS% MOD 8)
6345 FOR X = PNTS2% / 8 TO PNTS% STEP PNTS2% / 8
6351 IF ITEMS$ = "1" OR ITEMS$ = "4" OR ITEMS$ = "6" THEN
GOSUB 8800: REM x axis labelling in Ch. No.
6352 IF ITEMS$ = "4" OR ITEMS$ = "CAL6" THEN GOSUB 8700:
REM Upper x axis labelling in Ch. No.
6355 NEXT X

6360 PRINT #1, "PA"; 1000; 7500; "D11,0"; "LB"; "M.S.U.
PHYSICS"; " "; DATE$; " "; "Time: "; TIME$
6362 PRINT #1, "PA"; 1000; 7200; "D11,0"; "LB"; "FSS"; " "
6365 PRINT #1, "PA"; 1500; 7000; "D11,0"; "LB"; "P$"; " "
6367 IF ITEMS$ = "CAL6" THEN PRINT #1, "PA"; 2000; 6800;
"D11,0"; "LB"; "Peak isomer shift = "; IS; " mm/s "; " "
6370 GOSUB 10000
6371 GOSUB 10000
6380 IF ITEMS$ <> "PUB6" THEN PRINT #1, "PA 10000 3500
D10,1 LBCounts"; " "
6382 GOSUB 10000
6384 GOSUB 10000
6390 PRINT #1, "PA 400 3000 D10,1 LBPercent Absorption";
" "
6392 GOSUB 10000
6394 GOSUB 10000
6395 IF ITEMS$ = "1" OR ITEMS$ = "4" OR ITEMS$ = "6" THEN
GOTO 6440
6400 PRINT #1, "PA 3000 1400 D11,0 LBVelocity in mm/sec";
VELSTD$
6405 GOSUB 10000
6410 GOSUB 10000
6415 GOSUB 10000
6420 IF ITEMS$ <> "PUB6" AND ITEMS$ <> "4" THEN PRINT #1,
"PA 4000 6400 D11,0 LBChannel Number"
6425 GOSUB 10000
6430 GOSUB 10000
6435 GOSUB 10000: GOTO 7000
6440 PRINT #1, "PA 4000 1400 D11,0 LBChannel Number"
6450 GOSUB 10000
6460 GOSUB 10000
6470 GOSUB 10000

7000 REM Point or curve plotting routine, from 6186, 6435,
or 6470
7010 FOR X = T1% TO PNTS%
7020 IF ITEMS$ = "4" THEN GOTO 7030
7022 REM G(X), no interf. calibr.

```

```

7023 G(X) = 1000 + 8000 * (X - T1%) / (PNTS% - T1%)
7025 G(X) = INT(G(X))
7027 GOTO 7520

7030 REM G(X) for interferometer-calibrated points
7031 'print "At line 7031 P6 = "; P6
7040 REM The next line skips the laser data
7050 IF ((X - 16) / 16) = INT((X - 16) / 16) THEN X =
X + 1
7060 IF P6 - ABS(V(X)) >= 0 THEN G(X) = 5000 + INT(8000
* V(X) / F3)
7561 'print "At line 7561, X = "; X; ", V(X) = "; V(X);
", and G(X) = "; G(X)
7562 'while inkey$ = ""
7563 'wend
7070 GOTO 7520

7520 YF = Y(X) * CFB3 / B3: REM CFB3 = OldB3/YS (see
line 11410)
7530 M(X) = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (YF
- CFDN))
7532 NEXT X

7535 IF ITEMS$="1" OR ITEMS$="5" THEN PRINT #1,"SP4;":GOSUB
10000: REM Pen 4 for curve

7538 FOR X = T1% TO PNTS%: REM Plotting
7542 IF M(X) > 6000 OR M(X) < 2000 GOTO 7580
7550 IF G(X) < 1000 OR G(X) > 9000 THEN 7580
7560 IF ITEMS$ = "4" OR ITEMS$ = "4'" OR ITEMS$ = "6" OR
ITEMS$ = "CAL6" OR ITEMS$ = "PUB6" THEN PRINT #1, "PA";
G(X); M(X); "PD PU;": GOTO 7580: REM For points
7570 PRINT #1, "PA"; G(X); M(X); "PD"; : REM For curve
7580 NEXT X
7590 PRINT #1, "PU";

7592 REM Box drawing
7693 IF BOX$ = "DRAWN" THEN GOTO 7607
7597 PRINT #1, "PA 1000 2000 PR PD 0 4000 8000 0 0 -4000
-8000 0 PU PA;": REM Box drawing
7605 BOX$ = "DRAWN"
7607 PRINT #1, "SP0;"
7608 CLOSE #1: CLOSE #2
7610 IF ITEMS$ = "6" OR ITEMS$ = "CAL6" OR ITEMS$ = "PUB6"
THEN RETURN: REM to 2500
7630 ERASE YY, BB, ZZ, GG, AA, AREA!, LW!, NRG!: GOTO 70

8600 REM Subroutine from 6324 for lower x axis
labelling in mm/s
8610 I = 5000 + (8000 * (P6 - P2) / F3)
8620 IF I < 1000 OR I > 9000 THEN RETURN
8630 PRINT #1, "PA"; I; 2000; "PD"; I; 2100; "PU"
8640 PRINT #1, "PA"; I - 100; 1800; "D11,0"; "LB"; P6;
" "
8650 GOSUB 10000
8660 GOSUB 10000
8670 RETURN

8700 REM Subroutine from 6352 for upper x axis labelling
in Ch. No.
8710 I = 5000 + (8000 * (V(X) - P2) / F3): REM Same as
8905, but no "INT"
8720 IF I < 1000 OR I > 9000 THEN RETURN
8730 PRINT #1, "PA"; I; 6000; "PD"; I; 5900; "PU"
8740 PRINT #1, "PA"; I - 250; 6200; "D11,0"; "LB"; X;
" "
8750 GOSUB 10000
8760 GOSUB 10000
8770 RETURN

8800 REM Subroutine from 6351 for lower x axis
labelling in Ch. No.
8810 I = 1000 + (8000 * (X - T1%) / (PNTS% - T1%))
8820 IF I < 1000 OR I > 9000 THEN RETURN
8830 PRINT #1, "PA"; I; 2000; "PD"; I; 2100; "PU"

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```

8840 PRINT #1, "PA"; I - 100; 1800; "D11,0"; "LB"; X;
" "
8850 GOSUB 10000
8860 GOSUB 10000
8870 RETURN

```

```

8900 REM Collins' subroutine (unused) from line 6330
for lower x axis labelling in mm/s
8905 I = 5000 + INT(8000 * (V(X) - P2) / F3)
8910 IF I < 1000 THEN 8950
8920 IF I > 9000 THEN 8950
8930 PRINT #1, "PA"; I; 2000; "PD"; I; 2100; "PU";
8940 PRINT #1, "PA"; I - 100; 1800; "D11,0"; "LB"; P6;
" "
8945 GOSUB 10000
8946 GOSUB 10000
8950 P6 = P6 + P5
8970 RETURN

```

```

9000 RESTORE: REM Reading plotter codes
9005 FOR X = 1 TO 6
9010 READ K$
9020 PRINT #1, K$
9030 NEXT X
9040 RETURN
9050 DATA CHR$(27).CHR$(64);0:
9060 DATA CHR$(27).164;;17:
9070 DATA CHR$(27).N;19:
9080 DATA CHR$(27).J
9090 DATA IN;
9110 DATA DT

```

```

10000 FOR J = 1 TO 10000
10005 NEXT J
10010 RETURN

```

```

10050 FOR J = 1 TO 30000!
10060 NEXT J
10070 RETURN

```

```

10075 FOR J = 1 TO 1000
10080 NEXT J
10085 RETURN

```

```

10100 REM F10 key event handler from line 72
10110 LOCATE 25, 1:
10120 INPUT "Return to menu (yes, no)"; akey$
10130 IF akey$ = "Y" OR akey$ = "y" THEN ERASE YY, BB, ZZ,
GG, AA, AREA!, LW!, NRG!: GOTO 70
10140 LOCATE 25, 1: PRINT SPACES(78): REM Deletes prompt
10150 RETURN

```

```

10160 REM F5 key event handler from line 74
10165 PR = 1: RETURN

```

```

10175 REM error handler for FS$ (line 770)
10180 BEEP: PRINT " "; FS$; "
FILE NOT FOUND"
10185 PRINT " (F10 to return to
menu)"
10190 PRINT: RESUME 730

```

```

10200 REM error handler for DAT$ (line 2020)
10205 BEEP: PRINT " "; DAT$; "
FILE NOT FOUND"
10210 PRINT " (F10 to return to
menu)"
10215 PRINT: RESUME 2005

```

```

10225 REM error handler for READPK$ = STDFE$ (line 2605)
10230 BEEP: PRINT " "; READPK$;
" FILE NOT FOUND"
10235 PRINT " (F10 to return to
menu)"
10240 PRINT: IF EF$ = "E" OR EF$ = "e" THEN RESUME 12070

```

```

10245 PRINT: IF EF$ = "F" OR EF$ = "f" THEN RESUME 2105
10250 REM error handler for STDEUS$ (line 12605)
10255 BEEP: PRINT " "; STDEUS$;
" FILE NOT FOUND"
10260 PRINT " (F10 to return to
menu)"
10265 PRINT: RESUME 12050

```

```

10275 REM error handler for OPENing plotter (line 6183)
10280 CLS: LOCATE 9, 20
10285 BEEP: PRINT "Plotter not responding: check switch
box and connectors"
10290 RESUME 6095

```

```

10300 REM error handler for printer (line 126 and 1450)
10305 CLS: LOCATE 9, 20
10310 BEEP: PRINT " Printer not responding: check
paper, power switch, connectors, etc."
10315 PRINT " Press the p key
and RETURN when ready "
10317 PRINT: INPUT " (RETURN only if you don't want
the printer to record your operation)", PRINT$
10320 IF PRINT$ = "P" OR PRINT$ = "p" THEN RESUME
10321 IF PRINT$ = "" OR PRINT$ = "" THEN PR = 0: RESUME

```

```

10325 CLOSE #3: REM Error handling from line 2636
10340 PRINT: PRINT " FAULTY Fe
STANDARD RUN!"
10345 PRINT: PRINT " "; STDFE$; " shows "; N; " lines and
a total of "; NRPARAMS; " parameters."
10350 PRINT " Choose an Fe standard run with
4 or 6 lines."
10355 PRINT " Press F10 if you wish to
return to the menu"
10360 PRINT: PRINT: PRINT: CLOSE #3: GOTO 2410

```

```

11000 REM The y axis scales: REM from line 6210
11005 REM Setting the baseline to maximum counts
11030 MAXCNT = 0
11039 'print: print " At 11039 T1%, PNTS%, MINCNT,
MAXCNT = "; T1%; PNTS%; MINCNT; MAXCNT
11040 FOR I = T1% TO PNTS%
11045 'print "L i n e 1 1 0 4 5"
11050 IF Y(I) > MAXCNT THEN MAXCNT = Y(I)
11051 'print: print " For I = "; i; " ", Y(I) = ";
Y(I); " MAXCNT = "; MAXCNT
11052 'gosub 10050: gosub 10050: GOSUB 10050
11060 NEXT I

```

```

11065 IF REPEATSC$ = "Y" OR REPEATSC$ = "y" THEN GOTO
11500: REM from line 6220
11067 IF ITEMS$ = "4" OR ITEMS$ = "4," THEN B3 = MAXCNT
11068 'print "MAXCNT = "; MAXCNT
11069 MINCNT = MAXCNT
11070 'print: print " MINCNT = "; mincnt
11071 'gosub 10050: gosub 10050
11072 FOR I = T1% TO PNTS% STEP 16
11080 FOR J = I TO (I + 14)
11085 IF J > PNTS% THEN GOTO 11120
11090 IF Y(J) < MINCNT THEN MINCNT = Y(J)
11091 'print: print " For I = "; i; " and J = "; j; "
Y(J) = "; Y(J); " MINCNT = "; mincnt
11092 'gosub 10050: gosub 10050: GOSUB 10050
11100 NEXT J
11101 'print: print " For I = "; i; " and J = "; j; "
Y(J) = "; Y(J); " MINCNT = "; mincnt
11102 'gosub 10050: gosub 10050: GOSUB 10050
11110 NEXT I
11120 MAXCNT$ = STR$(MAXCNT): MINCNT$ = STR$(MINCNT)
11124 REM The next line strips the space added by STR$
from the left
11125 MAXCNT$ = RIGHT$(MAXCNT$, LEN(MAXCNT$) - 1): MINCNT$
= RIGHT$(MINCNT$, LEN(MINCNT$) - 1)
11130 MAXPNT% = INSTR(MAXCNT$, "."): MINPNT% =

```

```

INSTR(MINCNT$, ".")
11140 IF MAXPNT% = 0 THEN MAXEXP% = LEN(MAXCNT$) - 1 ELSE
MAXEXP% = MAXPNT% - 2
11150 IF MINPNT% = 0 THEN MINEXP% = LEN(MINCNT$) - 1 ELSE
MINEXP% = MINPNT% - 2

11170 IF MAXEXP% <> MINEXP% THEN GOTO 11250
11180 MAXDIG% = 1: MINDIG% = 1: J = 0
11185 WHILE MINDIG% = MAXDIG%
11190 J = J + 1
11200 MAXDIG% = VAL(MID$(MAXCNT$, J, 1)): MINDIG% =
VAL(MID$(MINCNT$, J, 1))
11210 WEND
11213 IF (MAXDIG% - MINDIG%) <= 1 THEN Q% = 4: GOTO 11225
11215 IF (MAXDIG% - MINDIG%) <= 2 THEN Q% = 3: GOTO 11225
11220 IF (MAXDIG% - MINDIG%) <= 4 THEN Q% = 2 ELSE Q% = 1
11225 YS = 10 ^ (MAXEXP% + 2 - J - Q%)
11230 CFUP$ = LEFT$(MAXCNT$, J + Q% - 1): CFUP =
VAL(CFUP$): CFUP = CFUP + 1
11240 CFDN$ = LEFT$(MINCNT$, J + Q% - 1): CFDN =
VAL(CFDN$): GOTO 11290
11250 REM Routine for wide count spread
11260 DIFF% = MAXEXP% - MINEXP%
11270 CFUP$ = LEFT$(MAXCNT$, DIFF% + 1): CFUP = VAL(CFUP$)
+ 1
11280 CFDN$ = LEFT$(MINCNT$, 1): CFDN = VAL(CFDN$)

11290 IUP = 5500: REM Highest tic on the right y axis
(counts)
11300 IDN = 2500
11305 REM IUP - IDN = 3000
11310 REM (IUP - IDN)/(CFUP - CFDN) = 3000/10 = 300
11315 IF ITEM$ = "PUB6" THEN GOTO 11400
11317 CFSTEP = (CFUP - CFDN)/4
11318 CFSTEP = INT(CFSTEP)
11320 FOR CF = CFDN TO CFUP STEP CFSTEP: REM Right y axis
(counts)
11325 I = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (CF -
CFDN))
11330 PRINT #1, "PA"; 8900; I; "PD"; 9000; I; "PU";
11340 PRINT #1, "PA"; 9020; (I - 10); "D11,0"; "LB";
(CF * YS); " "
11350 GOSUB 10000
11360 NEXT CF
11370 GOSUB 10000

11400 REM Left y axis (percent absorption)
11410 ABSNUP2 = 1 - (YS * CFDN / B3)
11413 IF ABSNUP2 <= .02 THEN ABSNUP3 = .02: GOTO 11470
11417 IF ABSNUP2 < .05 THEN ABSNUP3 = ABSNUP2: GOTO 11470
11420 ABSNUP3 = 0: K = 1
11430 WHILE ABSNUP3 = 0
11440 ABSNUP3 = (INT(ABSNUP2 * (10 ^ K))) / (10 ^ K)
11450 K = K + 1
11460 WEND
11470 ABSNSP = (ABSNUP3) / 4
11480 CFB3 = B3 / YS
11485 CFUP3 = (CFB3) * (1 - ABSNUP3)
11490 IUP3 = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (CFUP3
- CFDN))
11495 IF ABSNUP3 > .02 AND IUP3 > 2400 THEN ABSNUP3 =
ABSNUP3 + ABSNSP
11500 ABSN = 0
11510 WHILE ABSN <= ABSNUP3
11520 CF = (CFB3) * (1 - ABSN)
11530 I = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (CF -
CFDN))
11535 IF I > 5800 OR I < 2200 THEN 11570
11540 PRINT #1, "PA"; 1000; I; "PD"; 1100; I; "PU";
11550 PRINT #1, "PA"; 440; I; "D11,0"; "LB"; (100 *
ABSN); " "
11560 GOSUB 10000
11570 ABSN = ABSN + ABSNSP
11575 IF ABSNUP3 > .02 THEN ABSN = (CINT(100*ABSN))/100:
REM ABSN sometimes is ragged
11580 WEND

```

11590 GOSUB 10000

11600 RETURN REM to line 6290

12000 REM Eu standard

```

12010 IF STDEU$ <> "" THEN INPUT "Want to use the same Eu
and Fe standard runs for calibration"; REPEUSTD$
12030 IF REPEUSTD$ = "Y" OR REPEUSTD$ = "y" THEN GOTO
12090
12050 PRINT : PRINT "Name of Eu standard run for
calibrating v = 0"
12060 PRINT " ("; CHR$(34); "Enter"; CHR$(34); : INPUT
"if no calibration desired): ", STDEU$
12065 IF STDEU$ = "" THEN GOTO 2410
12066 READPK$ = STDEU$: GOSUB 12600
12068 CALIBREU = PEAK
12070 PRINT : PRINT "Name of Fe standard run for
calibrating the v scale"
12080 INPUT " (do not omit this): ", STDFE$
12090 PRINT : PRINT
12200 GOTO 2135

```

12600 REM Reading Eu peak position (from line 12066 or
2285)

```

12603 ON ERROR GOTO 10250
12605 OPEN READPK$ FOR INPUT AS #4
12606 ON ERROR GOTO 0
12610 JUNK$ = ""
12615 WHILE RIGHT$(JUNK$, 9) <> "DEVIATION"
12620 LINE INPUT #4, JUNK$
12621 WEND
12640 JUNK = 0
12645 WHILE JUNK <> 4
12650 INPUT #4, JUNK
12655 WEND
12683 INPUT #4, PEAK
12686 CLOSE #4
12687 RETURN

```

```

12900 PRINT: PRINT "This program can only process Eu and
Fe runs (press F10 to return to menu)"
12910 GOTO 2055

```

## **APPENDIX C - PERSONNEL SUPPORTED**

## PERSONNEL INVOLVED

Frederick W. Oliver  
Professor - Physics Department  
Principal Investigator.

Eugene Hoffman  
Assistant Professor -Physics Department  
Research Scientist  
Professor Hoffman was responsible for developing computer codes for plotting on a pc the data fit by the mainframe computer. He also assisted with many of the administrative duties of the grant.

Richard Lockhart  
Professor - Prince Georges Community College  
Research Scientist  
Professor Lockhart worked on the project during the summer of 1995. He was responsible for ordering equipment and setting up the laboratory for making superconducting compounds.

Christopher Brown  
Graduate student -UMCP  
Mr. Brown was responsible for assisting in the laboratory to make superconductng samples.

Dereje Seifu, Lecturer - Physics Department  
Research Associate  
Dr. Seifu, a theoretical physicist , worked on developing software for analyzing experimental data on the mainframe computer.

Zarfar Kureishy  
Research Associate  
Mr. Kureishy assisted with the many technical tasks associated with carrying out the objectives of the research.

The students below assisted with analyzing data, writing software, and preparing samples for experimental measurements.

Laura Gardner - Graduate student  
Aaron Bowman - Undergraduate student  
Grace Gregory - Undergraduate student  
Mia Nicholson - Undergraduate student  
Takisha Miller - Undergraduate student  
Lester Richardson - Undergraduate student  
Daryle Strickland - Undergraduate student  
Fritz Pierre - High school student



## APPENDIX D - FINANCIAL REPORT

# FINANCIAL STATUS REPORT

(Long Form)

(Follow instructions on the back)

<b>1. Federal Agency and Organizational Element in Which Report is Submitted</b> NATIONAL AERONAUTICS AND SPACE ADMINISTRATION (NASA)		<b>2. Federal Grant or Other Identifying Number Assigned By Federal Agency</b> NAG5-2375		<b>OMB Approval No.</b> 0348-0039	<b>Page</b> 1	<b>of</b> 1 pages																	
<b>3. Recipient Organization (Name and complete address, including ZIP code)</b> MORGAN STATE UNIVERSITY HILLEN ROAD AND COLDSRING LANE, BALTIMORE, MARYLAND 21239																							
<b>4. Employer Identification Number</b> 526002033		<b>5. Recipient Account Number or Identifying Number</b> 522128-0360		<b>6. Final Report</b> <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No		<b>7. Basis</b> <input type="checkbox"/> Cash <input checked="" type="checkbox"/> Accrual																	
<b>8. Funding/Grant Period (See Instructions)</b> From: (Month, Day, Year) 04/01/95		To: (Month, Day, Year) 03/31/96		<b>9. Period Covered by this Report</b> From: (Month, Day, Year) 04/01/95		To: (Month, Day, Year) 09/30/95																	
<b>10. Transactions:</b>		<b>I</b> Previously Reported		<b>II</b> This Period		<b>III</b> Cumulative																	
a. Total outlays		\$ 113,065.46		\$ 36,061.21		\$ 149,126.67																	
b. Refunds, rebates, etc.		-0-		-0-		-0-																	
c. Program income used in accordance with the deduction alternative		-0-		-0-		-0-																	
d. Net outlays (Line a, less the sum of lines b and c)		113,065.46		36,061.21		149,126.67																	
<b>Recipient's share of net outlays, consisting of:</b>																							
e. Third party (in-kind) contributions		-0-		-0-		-0-																	
f. Other Federal awards authorized to be used to match this award		-0-		-0-		-0-																	
g. Program income used in accordance with the matching or cost sharing alternative		-0-		-0-		-0-																	
h. All other recipient outlays not shown on lines e, f or g		-0-		-0-		-0-																	
i. Total recipient share of net outlays (Sum of lines e, f, g and h)		-0-		-0-		-0-																	
j. Federal share of net outlays (line d less line i)		113,065.46		36,061.21		149,126.67																	
k. Total unliquidated obligations						-0-																	
l. Recipient's share of unliquidated obligations						-0-																	
m. Federal share of unliquidated obligations						-0-																	
n. Total federal share (sum of lines j and m)						149,126.67																	
o. Total federal funds authorized for this funding period						226,150.00																	
p. Unobligated balance of federal funds (Line o minus line n)						\$ 77,023.33																	
<b>Program income, consisting of:</b>						-0-																	
q. Disbursed program income shown on lines c and/or g above						-0-																	
r. Disbursed program income using the addition alternative						-0-																	
s. Undisbursed program income						-0-																	
t. Total program income realized (Sum of lines q, r and s)						-0-																	
<b>11. Indirect Expense</b> <table style="width: 100%; border: none;"> <tr> <td colspan="5"> <b>a. Type of Rate (Place "X" in appropriate box)</b>  <input type="checkbox"/> Provisional <input type="checkbox"/> Predetermined <input type="checkbox"/> Final <input type="checkbox"/> Fixed         </td> </tr> <tr> <td style="width: 20%;"><b>b. Rate</b></td> <td style="width: 20%;">75%</td> <td style="width: 20%;"><b>c. Base S &amp; W</b></td> <td style="width: 20%;">\$69,790.00</td> <td style="width: 20%;"><b>d. Total Amount</b></td> <td style="width: 20%;">\$ 52,342.50</td> </tr> <tr> <td colspan="3"></td> <td><b>e. Federal Share</b></td> <td colspan="2">\$ 52,342.50</td> </tr> </table>							<b>a. Type of Rate (Place "X" in appropriate box)</b> <input type="checkbox"/> Provisional <input type="checkbox"/> Predetermined <input type="checkbox"/> Final <input type="checkbox"/> Fixed					<b>b. Rate</b>	75%	<b>c. Base S &amp; W</b>	\$69,790.00	<b>d. Total Amount</b>	\$ 52,342.50				<b>e. Federal Share</b>	\$ 52,342.50	
<b>a. Type of Rate (Place "X" in appropriate box)</b> <input type="checkbox"/> Provisional <input type="checkbox"/> Predetermined <input type="checkbox"/> Final <input type="checkbox"/> Fixed																							
<b>b. Rate</b>	75%	<b>c. Base S &amp; W</b>	\$69,790.00	<b>d. Total Amount</b>	\$ 52,342.50																		
			<b>e. Federal Share</b>	\$ 52,342.50																			
<b>12. Remarks:</b> Attach any explanations deemed necessary or information required by Federal sponsoring agency in compliance with governing legislation.																							
<b>13. Certification:</b> I certify to the best of my knowledge and belief that this report is correct and complete and that all outlays and unliquidated obligations are for the purposes set forth in the award documents.																							
Typed or Printed Name and Title Patrick M. O'Brien, Comptroller				Telephone (Area code, number and extension) (410) 319-3045																			
Signature of Authorized Certifying Official 				Date Report Submitted 12/6/95																			

# REQUEST FOR ADVANCE OR REIMBURSEMENT

Approved by OMR of Management and  
Budget, No. 80-R

PAGE 1 OF 1  
PAGES

(See instructions on back)  
1. FEDERAL SPONSORING AGENCY AND ORGANIZATIONAL ELEMENT TO  
WHICH THIS REPORT IS SUBMITTED  
NATIONAL AERONAUTICS AND SPACE ADMINISTRA-  
TION (NASA)

6. EMPLOYER IDENTIFICATION  
NUMBER

526002033

7. RECIPIENT'S ACCOUNT NUMBER  
OR IDENTIFYING NUMBER

522128-0360

8. RECIPIENT ORGANIZATION

Name: MORGAN STATE UNIVERSITY  
COMPTROLLER'S OFFICE

Number and Street: HILLEN ROAD & COLDSRING LA.

City, State and ZIP Code: BALTIMORE, MARYLAND, 21239

2. FEDERAL GRANT OR OTHER  
IDENTIFYING NUMBER ASSIGNED  
BY FEDERAL AGENCY  
NAG5-2375

3. PARTIAL PAYMENT REQUEST  
NUMBER FOR THIS REQUEST

9. PERIOD COVERED BY THIS REQUEST

FROM (month, day, year)

04/01/95

TO (month, day, year)

09/30/95

10. PAYEE (Where check is to be sent to different than item 8)

Name:

Number and Street:

SAME

City, State and ZIP Code:

## 11. COMPUTATION OF AMOUNT OF REIMBURSEMENTS/ADVANCES REQUESTED

PROGRAMS/FUNCTIONS/ACTIVITIES ▶	(a)	(b)	(c)	TOTAL
a. Total program outlays to date (As of date)	\$ 149,126.67	\$	\$	\$ 149,126.67
b. Less: Cumulative program income	-0-			-0-
c. Net program outlays (Line a minus line b)	149,126.67			149,126.67
d. Estimated net cash outlays for advance period	-0-			-0-
e. Total (Sum of lines c & d)	149,126.67			149,126.67
f. Non-Federal share of amount on line e	-0-			-0-
g. Federal share of amount on line e	149,126.67			149,126.67
h. Federal payments previously requested	113,065.46			113,065.46
i. Federal share now requested (Line g minus line h)	\$ 36,061.21			\$ 36,061.21
j. Advances required by month, when requested by Federal grantor agency for use in making prescheduled advances				
1st month				-0-
2nd month				-0-
3rd month				-0-

## 12. ALTERNATE COMPUTATION FOR ADVANCES ONLY

a. Estimated Federal cash outlays that will be made during period covered by the advance	\$ -0-
b. Less: Estimated balance of Federal cash on hand as of beginning of advance period	-0-
c. Amount requested (Line a minus line b)	\$ -0-

## 13. CERTIFICATION

I certify that to the best of my knowledge and belief the data above are correct and that all outlays were made in accordance with the grant conditions or other agreement and that payment is due and has not been previously requested.

SIGNATURE OF AUTHORIZED CERTIFYING OFFICIAL

*Patrick M. O'Brien*

TYPED OR PRINTED NAME AND TITLE

Patrick M. O'Brien, Comptroller

DATE REQUEST  
SUBMITTED

12/6/95

TELEPHONE (AREA  
CODE, NUMBER,  
EXTENSION)

(410) 319-3045

This space for agency use

# FEDERAL CASH TRANSACTIONS REPORT

(See instructions on the back. If report is more than one grant or assistance agreement, attach completed Standard Form 272-A.)

Is submitted NATIONAL AERONAUTICS AND SPACE ADMINISTRATION (NASA)

## 2. RECIPIENT ORGANIZATION

Name: MORGAN STATE UNIVERSITY  
 Number and Street: COMPTROLLER'S OFFICE  
 HILLEN ROAD & COLDSRING LANE

City, State and ZIP Code: BALTIMORE, MARYLAND 21239

3. FEDERAL EMPLOYER IDENTIFICATION NO. 526002033

4. Federal grant or other identification number: NAG5-2375  
 5. Recipient's account number or identifying number: 522128  
 6. Letter of credit number: N/A  
 7. Last payment voucher number: -0-  
 Give total number for this period  
 8. Payment Vouchers credited to your account: -0-  
 9. Treasury checks received (whether or not deposited): -0-

## 10. PERIOD COVERED BY THIS REPORT

FROM (month, day, year) 04/01/95 TO (month, day, year) 09/30/95

## 11. STATUS OF FEDERAL CASH

(See specific instructions on the back)

a. Cash on hand beginning of reporting period	\$ ( 37,308.46)
b. Letter of credit withdrawals	-0-
c. Treasury check payments	37,308.46
d. Total receipts (Sum of lines b and c)	37,308.46
e. Total cash available (Sum of lines a and d)	-0-
f. Gross disbursements	36,061.21
g. Federal share of program income	-0-
h. Net disbursements (Line f minus line g)	36,061.21
i. Adjustments of prior periods	-0-
j. Cash on hand end of period	\$ (36,061.21)

## 12. THE AMOUNT SHOWN ON LINE 11J, ABOVE, REPRESENTS CASH REQUIREMENTS FOR THE ENSUING

Days

## 13. OTHER INFORMATION

a. Interest income	\$ -0-
b. Advances to subgrantees or subcontractors	\$ -0-

## 14. REMARKS (Attach additional sheets of plain paper, if more space is required)

## 5. CERTIFICATION

I certify to the best of my knowledge and belief that this report is true in all respects and that all disbursements have been made for the purpose and conditions of the grant or agreement.

AUTHORIZED CERTIFYING OFFICIAL

SIGNATURE

TYPED OR PRINTED NAME AND TITLE

Patrick M. O'Brien, Comptroller

TELEPHONE (Area Code) 410 (Number) 319

DATE REPORT SUBMITTED

12/6/95

(Extension) 3045

## THIS SPACE FOR AGENCY USE